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Project Technical Report
of ISTC 2443p**

Monte Carlo Simulation of Plumes Spectral Emission

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**Institute for Problems in Mechanics Russian Academy of Sciences
(IPMech RAS)**

Director of IPMech RAS:

Felix Leonidovich Chernousko

Project Manager:

Sergey Timofeevich Surzhikov

**phone: (7-095) 433 82 98
fax: (7-095) 938 20 48
e-mail: surg@ipmnet.ru**

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Introduction

Objectives of the project

Methods of spectral diagnostics of nonhomogeneous volumes of heated gases are the most challenging for investigation of exhaust plumes of the hydrogen and carbon-hydrogen fuels. Computing methods of calculation of spectral heat radiation emissivity are the components of the general problem. The numerical simulation of plumes radiation is a challenging problem because there is a large number of different factors which characterize the phenomena of the spectral radiation transfer in the multiphase flows (for example: strong spectral dependence of the optical properties of heated and atmospheric gases, light-scattering processes, multi-dimensional character of the radiative energy transfer, phase transitions inside solid/liquid particles, thermodynamic nonequilibrium, etc.).

This scientific direction is very significant for aerospace applications and for purposes of the ecological monitoring.

There have been many previous computational simulations of liquid and solid rocket motor plumes radiation signatures using a wide range of computational methods and models, for example:

1. Simmons, F.S., Rocket Exhaust Plume Phenomenology. The Aerospace Press, 2000, 286 p.
2. Ebrahimi, H.B, Kawasaki, A., “Numerical Investigation of Exhaust Plume Radiative Transfer Phenomena,” AIAA-98-3623, 1998.
3. Wright, M.J., Rao, R.M., Candler, G.V., Hong, J.S., Schilling, T.A., Levin, D.A., “Modelling Issues in the Computation of Plume Radiation Signature,” AIAA 98-3622, 1998.
4. Simmons, M., “The Integration of CFD Modeling and Simulation into Plume Measurement Programs,” AIAA-99-2255, 1999.
5. Rao, R.M., Sinha, K., Candler, G.V., Wright, M.J., Levin, D.A., “Numerical Simulation of Atlas II Rocket Motor Plumes,” AIAA-99-2258, 1999.
6. Alexeenko, A., Collins, R., Gimelshein, S., Levin, D.A., Hong, J., Schilling, T., “Modeling of Radiation in the Atlas Plume-Flow,” AIAA-2001-0355, 2001.

7. Surzhikov, S.T., Howell, J.R., “Monte Carlo Simulation of Radiation in Scattering Volumes with Line Structure,” Journal of Thermophysics and Heat Transfer, 1998, Vol.12, No.2, pp.278–281.

Common fault of listed papers is use of approximate calculation methods for representation of spectrum structure of the heat radiation. This is due to extremely high labour-intensiveness of the spectral problem solution procedure.

Together with it, there is a large practical need for new methods of calculation of selective radiation heat transfer, allowing to take into account rotary structure of a molecular spectrum. Also it is necessary to provide a capability of comparative analysis of different methods, in particular: the line-by line methods, statistical simulation methods (these methods are based on the **Monte-Carlo methods**), statistical models of a molecular spectrum. There is a need also in creation of the new computational methods using new computer technologies (for example, **parallel computing algorithms**).

Development of the numerical simulation methods and codes for prediction of spectral directional emissivity, especially those based on Monte-Carlo random simulation, demands formulation and a priory justification of the following basic scientific problems:

1. Creation and testing of the "elementary" one-, two-, and three dimensional (1D, 2D, 3D) benchmark problems intended for **verification** computing codes being made for prediction spectral signatures of exhaust plumes;
2. Creation of Monte-Carlo simulation codes considering linear fine structure of molecular spectra at plumes spectral visibility predictions through thickness of cold atmosphere (so-called the “Hot/Cold” problem of radiation transfer);
3. Numerical study of different approaches for calculation average parameters of Band models (intensities, half-widths) for “Hot/Cold” problems;
4. Modification of Random Band models for taking into account scattering processes.

Being developed these methods and codes should be used for numerical simulation of the 2D benchmark and real problems for real atmospheric parameters. It will give possibility to analyze different optical models of hot and cold atmosphere, such as: line-by-line model (HITRAN database), different random models. This analysis should also take into account available experimental data.

And the last general goal of the project is creation of Database of Molecular Lines for prediction spectral, narrow-band and wide-band visibility of heated gas volumes in real atmosphere by Monte-Carlo methods.

Expected results

The project will achieve the following tangible results:

- 1) The following computing codes for calculation of the spectral emissivity of nonhomogeneous light-scattering plumes by the Ray Tracing Monte-Carlo method will be created:
 - a) Computing code **LBL-SRT-RTMC** for “Line-by-Line” calculations;
 - b) Computing code **SRT-RTMC-NSM** intended for narrow band Spectral Radiation Transfer Ray Tracing Simulation by the Monte-Carlo method with regard to the Narrow Band Statistical Model of molecular lines;
 - c) Computing code **SRT-RTMC-WSM** intended for wide band Spectral Radiation Transfer Direct Simulation by the Monte- Carlo method with regard to the Wide Band Statistical Model of molecular lines,
 - d) Computing code **IRT-RTMC-MSM** intended for Integral Radiation Transfer Direct Simulation by the Monte Carlo method with regard to the Macro-Random Statistical Model of vibrational molecular bands;
- 2) 3D computing codes for prediction of plumes spectral emissivity based on the Monte-Carlo method will be created. This code will use the following models of the molecular lines spectrum:
 - a) the model **LBL-SRT-RTMC** for “Line-by-Line” calculations;
 - b) the model **SRT-RTMC-NSM** intended for narrow band Spectral Radiation Transfer.
- 3) Electronic data base on spectral optical properties of exhaust gases will be created;
- 4) Series of systematic numerical investigations pertinent to different numerical simulation schemes of the Monte-Carlo imitation algorithms with reference to radiation transfer in light-scattering rocket exhausts will be performed;
- 5) Publication of general results of the investigation (AIAA papers, etc.).

This project has a basic research character, because computing models and codes, which will be created may be used not only for aerospace applications but also for astrophysics, optics of atmosphere, physics and chemistry of the low-temperature plasma, etc.

Technical Approach

All computing codes being developed are based on the different Ray Tracing Monte-Carlo (RTMC) algorithms combined with different models of fine rotational line structure of molecular spectrum.

Mathematical technology of parallel computation will be applied for the developing codes. The codes will be written on the base of FORTRAN-90 for Digital FORTRAN 6.5 with using MPICH/MPI software

For prediction of optical properties of heated gases the HITRAN Data Base (Air Force Geophysical Lab.) and the ASTEROID computing system (this is new version of code MONSTER developed by Prof. S.T. Surzhikov) will be used.

I. Summary of Project Technical Report

All expected results have been achieved in full measure. Brief description of the results are presented below.

Task 1 (the first year of the project)

The following algorithms of statistical simulation of radiation heat transfer which are based on the use of the ray tracing method of photon trajectories (the Monte-Carlo simulation method) were studied at the first stage of the project:

1. Line by line integration;
2. Hybrid statistical model;
3. Method of smoothing coefficients;
4. Two-group method;
5. Line by line integration with little number of trajectories;
6. Inverse simulation algorithms;
7. Fast algorithm for calculation parameters of optical path.

The general purpose of the stage was the study of listed algorithms and their comparative analysis, based on the results of radiation transfer simulation in flat and cylindrical scattering volumes containing molecules with line absorption of thermal radiation.

Some new accelerating modifications of the algorithms were studied at the first stage. It has been shown that the calculation efficiency of the Ray Tracing Monte-Carlo method can be somewhat improved by using “weighting” algorithms. In our case, the following modification of studied algorithms was used:

- a) Each photon being simulated in the initial state was assigned a certain amount of energy (the term “photon” is to be taken conventionally: we are dealing with a quasi-particle being simulated, which possesses the main properties of a photon beam);
- b) The photon trajectory was not terminated in the case of an absorbing collision, but its energy decreased in accordance with the law of exponential decay;
- c) The trajectory was simulated until the photon energy became less than the preassigned value (for example, 10^{-5} of the initial energy) or until the photon left the calculation region.

- d) Studied numerical simulation algorithms were presented in Papers [1, 2] at AIAA conferences.

Task 2 (the first year of the project)

The following algorithms of statistical simulation of radiation heat transfer which are based on the use of Monte-Carlo ray tracing methods were developed for arbitrary non-orthogonal grids:

1. Line by line integration;
2. Hybrid statistical model;
3. Method of random sampling of photon trajectory parameters.

Comparison of numerical simulation results obtained by developed Monte-Carlo algorithms on orthogonal and non-orthogonal calculation grids was performed. It is shown that these algorithms give the same numerical simulation results for identical distribution of thermo-gas-dynamic parameters in model plumes.

Studied numerical simulation algorithms were presented at summer AIAA'2004 Thermophysics conference. Results of this stage were published in AIAA paper No. 2003-3895.

Task 3 (the first year of the project)

Computing code **LBL-SRT-RTMC** intended for the line-by-line calculation of spectral radiation heat transfer by the ray tracing Monte-Carlo method in narrow bands of molecular lines has been developed. This is general computing code within the project 2443, which will be used for benchmark calculations of spectral directional emissivity.

This computing code is based on the HITRAN-like representation of the molecular lines parameters. In particular, the HITRAN database [Rothman, L.S., Gamache, R.R., Tipping, C.P. et al. "The HITRAN molecular database: Edition of 1991 and 1992," JQSRT, 1992, Vol.48, No.5/6, pp.469–507] was used for calculation of spectral directional emissivity of model plumes in centers of vibrational bands (where the use of HITRAN database is acceptably [Surzhikov, S.T., "Spectral and Narrow Band Directional Emissivity of Light-Scattering and Non-Scattering Volumes," AIAA paper 2002-3324, 2002, 21 p.]). The numerical study was performed for different vibrational-rotational bands of H₂O, CO₂, CO molecules.

Systematical study of the developed code was performed both for the non-scattering and scattering 2D volumes. Multi-temperature poly-disperse heterogeneous plumes, and orthogonal and non-orthogonal calculation grids were used for these calculations.

Task 4 (the first year of the project)

Computing code **SRT-RTMC-NSM** intended for the narrow band calculation of spectral radiation transfer through non-homogeneous gas volumes by the Monte-Carlo ray tracing method with regard to the Narrow Band Statistical Model of molecular lines was created and investigated.

Numerical study of the developed code was performed both for the non-scattering and scattering 2D volumes. Different types of the Narrow Band Statistical models have been investigated. Numerical study of the developed method has been performed on the example of the multi-temperature poly-disperse heterogeneous plumes.

Task 5 (the first year of the project)

Computing code **SRT-RTMC-WSM** intended for the wide band calculation of spectral radiation transfer through non-homogeneous gas volumes by the Monte-Carlo ray tracing method with regard to the Wide Band Statistical Model of molecular lines was created and investigated.

Numerical study of the developed code was performed both for the non-scattering and scattering 2D volumes. Different types of the Wide Band Statistical models have been investigated. Numerical study of the developed method has been performed on the example of the multi-temperature poly-disperse heterogeneous plumes.

Task 6 (the first year of the project)

Computing code **SRT-RTMC-MSM** intended for calculation of integral radiation transfer through non-homogeneous gas volumes by the Monte-Carlo ray tracing method with regard to the Macro Random Model of molecular lines was created and investigated.

Numerical study of the developed code was performed both for the non-scattering and scattering 1D volume. Numerical study of the developed method has been performed on the example of the multi-temperature poly-disperse heterogeneous medium.

Task 7 (the first year of the project)

Computing codes for random (Monte-Carlo) simulation of molecular lines with reference to a problem of radiation transfer through very inhomogeneous optical paths have been developed. These codes were developed on the base of some modifications of the Curtis – Godson models.

Developed codes were included in codes, developed at earlier stages of the Project 2443p: **SRT-RTMC-NSM** and **SRT-RTMC-WSM**.

To estimate accuracy of developed codes, which take into account specificity of very inhomogeneous optical paths, the code **LBL-SRT-RTMC** was modified. This code is intended for “Line-by-Line” calculations, therefore any inhomogeneity can be described inside the code without additional modifications. But at these calculations one needs more precise describing of inhomogeneous regions in calculation domain. Therefore a special algorithm for numerical simulation on extremely inhomogeneous grids was developed and tested.

Preliminary numerical simulation results were obtained by all developed codes for non-scattering media. It was shown that developed models allow predict integral signature of non-scattering model plumes (gasdynamic parameters of which were described at previous stages of the project) with relative accuracy about 30%.

Task 8 (the first year of the project)

Numerical simulation code for prediction of fluctuating gasdynamic parameters of model plumes has been developed. The code realizes two opposite physical models of possible local gasdynamic fluctuations: the model of coherent (fully correlated) fluctuations, and the model of un-coherent fluctuations (un-correlated fluctuations). In the last case a distribution function for gasdynamic fluctuations has the local-Gaussian form. Typical time scale of the fluctuations in the both cases corresponds to average life-time of large scale vortexes, which are generated in plumes.

Theoretical study of effect of gas dynamic parameters fluctuation on integral emissivity of homogeneous (non-scattering) plumes was performed. It was shown that gasdynamic fluctuations (first of all, temperature fluctuations) within the limits ~10% provide uncertainties in integral directional emissivity of model plumes within the limits ~25%.

Task 9 (the first year of the project)

Computing model for numerical simulation of the three dimensional spectral signatures of rocket exhaust plumes by the ray tracing Monte-Carlo method was developed. The model includes proper of the ray tracing Monte-Carlo algorithms and it is consisted with spectral methods for interpretation of molecular lines fine structure of emitting spectra.

Numerical simulation results for sunlight scattering on high-altitude space vehicle plume and for three-dimensional plume of heavy launch vehicle were obtained and published.

Task 10 (the first year of the project)

MPICH software was installed on personal computers (4 Pentium-IV processors, 2.6 GHz). MPICH is a portable implementation of the full MPI-1.2 specification for a wide variety of parallel and distributed computing environments, where MPI (Message-Passing Interface) is a standard specification for message-passing libraries. MPICH contains, along with the MPI library itself, a programming environment for working with MPI codes. The programming environment includes a startup mechanism and a profiling library for studying the performance of MPI programs.

As the first stage of analysis of possibility to use parallel computing algorithms for developed computational codes, which are realize Monte-Carlo algorithms, a trivial distribution of calculation processes between available processors has been realized. It was shown, that at simulation of 10^6 photon groups for typical calculation case (with scattering) speed up of the calculations achieves value of 7.95 times.

Task 1 (the second year of the project)

Formulation and a priory justification of “elementary” 1D, 2D, 3D benchmark problems intended for verification computing codes were performed for prediction spectral signatures of exhaust plumes by Monte-Carlo methods. Verification of ray tracing Monte-Carlo algorithms, which are used in the code **Plume-2D-MC** has been performed. For these purposes a special succession of the benchmark problems has been developed for verification computing codes based on ray tracing Monte-Carlo methods. This succession of the benchmark problems is recommended for further development of different radiation heat transfer methods and codes.

The problem of code verification was discussed at summer (2005) AIAA Thermophysics conference and published in Ref.1.

Task 3 (the second year of the project)

Numerical simulation of the 2D benchmark problems for real atmospheric parameters has been performed. Analysis of different optical models of atmosphere: line-by-line model (HITRAN database), random models with different algorithms of averaging of rotational lines has been performed. Analysis and numerical interpretation of ERIM experimental data [Lindquist G.H., Arnold C.B., Spellicy R.L. Atmospheric Absorption Applied to Plume Emission. Experimental and Analytical Investigations of Hot Gas Emission Attenuated by Cold Gases. Report ERIM No. 102700-20-F, AFRPL-TR-75-30. August 1975, 208 p.] has been performed. The code **Plume-2D-MC**, which realizes several Monte-Carlo simulation algorithms developed in the previous stages of the project, and several spectral optical models of heated gases (the NASA standard infrared model, the HITRAN database, the CDSD-1000 database, some analytical semi-empirical wide-band models, and analytical semi-empirical wide/narrow models) has been used for these purposes.

Task 4 (the second year of the project)

Database of Molecular Lines for prediction spectral, narrow-band and wide-band visibility of heated gas volumes in real atmosphere by Monte-Carlo methods has been created and has been included into ASTEROISD code. These databases were used in the code **Plume-2D-MC**.

Task 5 (the second year of the project)

Description of source texts of developed computing code **Plume-2D-MC** has been performed. This computing code is intended for prediction of spectral directional emissivity (spectral signature) of heated gas volumes, and for prediction of an attenuation of the heat radiation by long paths of cold atmospheric gases. This computing code is based on codes **LBL-SRT-RTMC**, **SRT-RTMC-NSM**, **SRT-RTMC-WSM** developed at the first stage of the

project. The code description and its FORTRAN-text have been delivered to the partner organization. A description of several calculation test cases, which can be used for verification of code **Plume-2D-MC** has been performed and attached to the code description. The descriptions of the each calculation test case are accompanied by separate directories inside general directory **Plume-2D-MC-Hybrid**. These directories contain initial conditions for the given calculation test (in directory **INPUT_Data**) and graphical representation of corresponding numerical simulation results (in directory **RESULTS**).

A recommendation for including of the any new optical models into the calculation code **Plume-2D-MC** has been prepared.

One of significant scientific results obtained in the project is the reasonable prediction of ERIM experimental data of hot gas cells radiance, both unattenuated and attenuated by long atmospheric paths. The work was performed in compliance with additional agreement between IPMech RAS and Partner organization (June 2005, Toronto, Canada). Figure 1 (see Attachment 1) shows example of comparison of experimental data ERIM and numerical simulation prediction obtained by code **Plume-2D-MC**.

II. Description of code **Plume-2D-MC**, intended for prediction of spectral signature of plumes by the Monte-Carlo method

Introduction

The part II.1 of the technical report presents source texts of computing code **Plume-2D-MC**. This computing code is intended for prediction of spectral directional emissivity (spectral signature) of heated gas volumes, and for prediction of an attenuation of the heat radiation by long paths of cold atmospheric gases.

The code **Plume-2D-MC** has been wrote with the use of FORTRAN-77 standard programming language. In accordance with the conditions of the project #2243p (the first part of the project) this code has been used under Microsoft operating system. The Compaq Visual Fortran Professional Edition 6.5.0 (Compaq Computer Corporation) and Techplot Version 10.0-0-7 (Amtec Engineering, Inc.) were used for calculation and graphical representation of numerical simulation results.

The code **Plume-2D-MC** realizes several Monte-Carlo simulation algorithms, which were developed in the previous stages of the project, and several spectral optical models of heated gases (the NASA standard infrared model, the HITRAN database, the CDSD-1000 database, some analytical semi-empirical wide-band models, and analytical semi-empirical wide/narrow models).

This part of the technical report presents also results of study of mathematical accuracy of imitating Monte-Carlo algorithms, which are used in the code **Plume-2D-MC**, and it contains results of numerical predictions of ERIM experimental data [2] of hot gas cells radiance, both unattenuated and attenuated by long atmospheric paths.

The part II.2 contains description of several calculation test cases, which can be used for verification of code **Plume-2D-MC**. Description of the each calculation test case is accompanied by separate directory inside general directory **Plume-2D-MC-Hybrid**, containing initial conditions for the given calculation test (in directory **INPUT_Data**) and graphical representation of corresponding numerical simulation results (in directory **RESULTS**).

The part II.3 contains recommendations for including of the new optical models into the code.

The report contains brief description of the code structure (Appendix 2 of the report), which can help in adaptation of the code on other operating systems and other computers.

In accordance with the interim agreement between Partner-Organization and IPMech RAS (June 2005, Toronto, Canada), and also in accordance with e-mail letter (e-mail of July 12, 2005, signed by Dr. I. Wysong) the report contains answers on all questions formulated in the e-mail. But, of course, not all of planned tasks have been solved and presented in the report, because large part of the work (especially on spectral optical models and on numerical simulation algorithms, taking into account rotational line structure in conditions of light-scattering) are planned on the second year of the project (for the period October, 2005 – September, 2006).

It should be noted especially, that presented results of the code verification show only small part of potential possibilities, which are included in the code. Presented code **Plume_2D_MC** and recently created code **Plume_3D_MC** allow solve many problems of practical interest on prediction of spectral radiance of localized in space heated volumes. However, the problem of co-ordination of the radiation heat transfer simulation code and available databases of spectral optical properties (or new calculation models of spectral optical properties) should be solved in the future.

II.1. Code Plume-2D-MC verification.

Numerical prediction of ERIM experimental data

Systematization of test problems of the theory of radiation heat transfer, which are used in the given report for testing computing models LBL-SRT-DSMC (the Line-by-Line Spectral Radiation Transfer by Direct Simulation Monte-Carlo) and SRT-DSMC-NSM (the Spectral Radiation Transfer by Direct Simulation Monte-Carlo Narrow Spectral Models), is submitted in Ref.1. These numerical simulation models are realized in computing code **Plume-2D-MC**. In order to increase reliability of numerical data predicted by the code Plume-2D-MC, a novel computing code Plume-3D-MC was also used. The last code realizes algorithms of integral estimation (MCIEDE – Monte-Carlo Integral Estimation of Directional Emissivity) and algorithm of local estimation (MCLEDE – Monte-Carlo Local Estimation of Directional Emissivity). The specified computing codes have been subjected to multilevel testing.

The following problems of radiation heat transfer were solved by the developed computing codes:

1. Prediction of radiance of homogeneous gray non-scattering plane layer (the Problem I);
2. Prediction of directional radiating ability of homogeneous volumes of grey volume of spherical and cylindrical forms (the Problems II and III);
3. Prediction of spectral directional radiating ability of homogeneous volumes of heated gases H_2O and CO_2 (the Problem IV): interpretation of the ERIM experimental data on hot cell radiance;
4. Calculation of spectral intensity of radiation of homogeneous volumes of heated gases H_2O and CO_2 , which is registered by radiation detector located on significant distance from the radiating volume (the Problem V): interpretation of the ERIM experimental data on “hot-through-cold” cell radiance.

Results of the testing are presented in the report.

Problem I.

Prediction of normal heat radiation intensity of homogeneous layer of grey non-scattering medium

Schematic of the problem is shown in Fig. 1.

This problem has the following exact analytical solution

$$J_{\omega} = J_{b,\omega} [1 - \exp(-\kappa_{\omega}H)], \quad (1)$$

where J_{ω} is the spectral radiation intensity; $J_{b,\omega}$ is the spectral intensity of black body (the Planck function); κ_{ω} is the spectral absorption coefficient (in the given case this coefficient is assumed as constant); H is the depth of the plane layer.

Let $H = 60$ cm, $\kappa = 1/H$, $J_{b,\omega} = 1$. Then, from Eq.(1) : $J_{\omega} = 0.63212$.

Numerical simulation results for spectral radiation intensity of a flat layer in a normal direction obtained with the use of code **Plume-2D-MC** are shown in Figs. 2-5. The homogeneous cylindrical volume imitates the plane layer in the given case. Height of the volume is $H = 60$ cm, and its radius is $R_c = 100$ cm. Heat radiation signature S_{\perp} of the cylindrical volume in the

normal to planes $x=0$ and $x=H$ directions was predicted. The spectral intensity was calculated as follows

$$J_{\perp} = \frac{S_{\perp}}{\pi R_c}.$$

The problem was resolved in a “gray” statement, when the spectral absorption coefficient κ_{ω} does not depend on radiation wavenumber. But the numerical simulations were carried out in sixty spectral sub-regions on the spectral region $\Delta\Omega=3000\div4400\text{ cm}^{-1}$. It allowed graphically show statistical errors: the oscillations of numerical simulation data in Figs.2-5 are conditioned just by the statistical errors of the numerical simulation.

To receive quantitative characteristics of the statistical errors, the series of numerical experiments with different number of simulated photons has been executed (see Table 1)

Table 1

Calculation series	N_{ph}	$\varepsilon, \%$	Figure
1	10^5	11.0	2
2	10^6	4.9	3
3	10^7	0.6	5

The relative error ε was calculated with respect to the mean value $J=0.618$. Difference between the mean value $J=0.618$ and the precise value $J=0.63212$ is accounted by the finite different discretization of angular space for each simulating photon. To illustrate the kind of errors, special numerical simulation experiments were performed at $N_{\theta}=21$, $N_{ph}=10^6$, where N_{θ} is the number of angular zones from $\theta=0$ up to $\theta=\frac{\pi}{2}$ (see Fig.4). Numerical simulation results obtained at $N_{\theta}=41$ are shown in Figs. 2, 3, 5 (see Table 1).

Comparing results of numerical simulation presented in Figs.3 and 4, it is possible to conclude the following:

1. Mean level of predicted intensity decreases with decreasing of N_θ (it means that the error of determination of mean intensity increases);
2. Statistical error decreases with decreasing of N_θ .

So, the algorithm MCIEDE has the following significant calculation properties:

1. Statistical errors of numerical simulation increases as number of zones of angular space discretization increases. This is because each elementary solid angle contains smaller number of photons.
2. Statistical errors decreases with decreasing of number of angular zones, but at the same time, the errors of prediction of mean value of intensity increase.

Therefore, there is necessity to perform additional numerical experiments for optimization of the errors in each calculation case.

Presented numerical simulation results give also additional information about statistical errors of the calculations.

Each of Figures 2–5 shows two spectral intensities. One of them corresponds to surface $x=0$, and other corresponds to surface $x=H$. In the conditions under consideration, these two intensities must be equal (due to symmetry of space). Differences between curves, which one can see at these figures are due to statistical errors.

Numerical simulation results predicted by code Plume-2D-MC show that relative errors of $\sim 1.9\%$ in determination of mean value of spectral intensity, at statistical error of $\sim 4.9\%$, can be achieved at number of simulating trajectories of $\sim N_{ph} = 10^6$.

As it was mentioned above, an additional verification of the numerical simulation results was performed with using three-dimensional code Plume-3D-MC. Spectral radiation intensities of the homogeneous plane layer of non-scattering gray medium are shown in Figs.6-9. The problem was solved in the following statement. A homogeneous cube was considered. A square of the cube side is equal $F = 10^4 \text{ cm}^2$. Spectral signature in a normal direction to each side was calculated with the use of the MCLEDE algorithm for each side of the cube. Division of the spectral signature by square of the cube side F yields the spectral radiation intensity.

A quantitative estimation of statistical errors of MCLEDE algorithm is presented in Table 2.

Table 2

Calculation series	N_{ph}	$\varepsilon, \%$	Figure
1	5×10^3	0.475	6
2	10^4	0.316	7
3	10^5	0.158	8
4	10^6	0.0317	9

From this table we notice that the MCLEDE algorithm gives mean value of spectral radiation intensity with relative errors of $\sim 0.0158 \%$, at level of statistical error of $\sim 0.475 \%$, even at low number of simulating trajectories ($N_{ph} = 5000$). In addition, it is obviously, that so little number of simulating trajectories leads to drastically decrease of calculation time.

Problem II.

Prediction of directional radiation ability (signature) of homogeneous non-scattering spherical volume

Codes Plume-2D-MC and Plume-3D-MC were used for solution of the problem. In the first case (the code Plume-2D-MC) a sphere of radius $R_{sph} = 30$ cm was located in the center of cylindrical volume of radius $R_{cyl} = 100$ cm and height $H_{cyl} = 200$ cm (see schematic of the problem in Figs.10,11). It is assumed that the absorption coefficient not being zero at temperature $T > 500$ K. Its value is equal to $\kappa = 0.01 \text{ cm}^{-1}$. The spectral intensity of black body corresponds to temperature 1200 K and given wavenumber from spectral region $\omega = 3000 \div 4400 \text{ cm}^{-1}$. The following calculation grid was used: $NI = 61$ (NI is the number of nodes along radial variable), $NJ = 121$, $N_\theta = 21$.

Numerical simulation results for spectral signature of the spherical volume from the side of cylindrical surface are shown in Figs.12, 13. It was assumed in the first case (Fig.12) that $N_{ph} = 10^5$, and in the second case $N_{ph} = 10^6$. Referring to Fig.12 it will be observed that statistical errors achieve of $\sim 2.7 \%$, and from Fig.13 we notice that the statistical errors achieve of $\sim 0.45 \%$.

Numerical simulation results for spectral signature of the spherical volume from the sides of plane surfaces are shown in Figs.14 and 15. One can see that statistical errors decrease from

$\sim 9.5\%$ to $\sim 1.9\%$ at increasing of number of simulating trajectories from $N_{ph}=10^5$ to $N_{ph}=10^6$.

The systematic errors $\sim 5\%$ between mean values of the signatures observed from cylindrical and plane surfaces is attributable to discretization errors in spatial and angular spaces for used cylindrical calculation domain.

As before, spectral signatures of the sphere predicted on two planes $x=0$ и $x=H$ give additional representation about statistical errors of Monte-Carlo simulation, because these spectral distributions should be equivalent.

Schematic of the problem, which is used for code Plume-3D-MC is shown in Figs.16 and 17. Typical numerical simulation results for any direction of observation are shown in Fig. 18. These calculations were carried out with the use of MCLEDE algorithm, at $N_{ph}=10^4$. It is evident from this figure that statistical error of the calculations close to $\sim 0.0149\%$. As before, the systematic discrepancy $\sim 4.2\%$ between the numerical simulation results obtained by Plume-2D-MC and Plume-3D-MC codes is due to finite difference discretization of spatial and angular spaces. It should be stressed that low level of statistical errors observed for code Plume-3D-MC at $N_{ph}=10^4$ is connected with using MCLEDE algorithm. If at the same number of simulating trajectories ($N_{ph}=10^4$) to use MCIEDE algorithm, the numerical simulation results will be much worse (see Figs.19 and 20). It is evident from the figures that accuracy of such prediction is very low.

Problem III.

Prediction of directional radiation ability (signature) of homogeneous non-scattering cylindrical volume

As before, codes Plume-2D-MC and Plume-3D-MC were used for solution of the problem. In the first case (code Plume-2D-MC) a heated cylindrical volume of radius $R_{hc}=30$ cm and height of $H_{hc}=60$ cm was located in the center of cylindrical computation domain of radius $R_{cyl}=100$ cm and height of $H_{cyl}=200$ cm (see schematic of the problem in Figs. 21, 22). It is assumed that the absorption coefficient not being zero at temperature $T > 500$ K. Its value is equal

to $\kappa = 0.01 \text{ cm}^{-1}$. The spectral intensity of black body corresponds to temperature 1200 K and given wavenumber from spectral region of $\omega = 3000 \div 4400 \text{ cm}^{-1}$. The following calculation grid was used: $NI = 61$ (NI is the number of nodes along radial variable), $NJ = 121$, $N_\theta = 21$. The spectral signature of the hot cylindrical volume is predicted for the following three directions $\theta = 0^\circ$, $\theta = 90^\circ$, and $\theta = 180^\circ$ (from the side of plane surfaces $X = 0$ and $X = H_{cyl}$, and from the side of cylindrical surface).

Spectral signature of cylindrical surface is shown in Fig.23. Statistical error achieves in this case of $\sim 3.6 \%$.

Spectral signatures of plane surfaces are shown in Fig.24. Statistical error achieves in this case of $\sim 3.1 \%$.

Three-dimensional calculations of spectral signatures were executed using Plume-3D-MC code. Schematic of the problem for this calculation case is shown in Figs.25–27. An algorithm of the local estimation (MCLEDE) was used in this case.

Spectral signature of the cylindrical volume from the side of cylindrical surface ($\theta = 90^\circ$) is shown in Fig.28, and spectral signature of plane surface ($\theta = 0^\circ$) is shown in Fig.29. Reference to Figs.28 and 29 shows that statistical error very low in these cases ($\sim 0.014 \%$).

Relative error of spectral signature prediction from the side of cylindrical surface by codes Plume-2D-MC and Plume-3D-MC achieves of $\sim 4.3 \%$, and relative error of spectral signature prediction from the side of plane surface achieves of $\sim 1.8 \%$.

From these numerical experiments on spectral signature prediction for heated volumes of simplest geometries some general conclusions can be drawn regarding codes Plume-2D-MC and Plume-3D-MC:

- 1) These codes allow predict spectral signatures with relative accuracy of $\sim 5 \%$ and with statistical errors about $\sim 5 \%$.
- 2) The algorithm MCLEDE, which is realized in code Plume-3D-MC, provides low levels of errors in the region of $\sim 0.04\%$, at statistical error of $\sim 0.05\%$. The method provides a high performance of computation.

Problem IV.

Prediction of spectral signature of homogeneous non-scattering cylindrical volumes, containing mixtures ($\text{H}_2\text{O}/\text{N}_2$) и (CO_2/N_2) at high temperatures. Interpretation of experimental data [2] with the use of codes Plume-2D-MC and Plume-3D-MC

Schematic of the problem is shown in Figs. 30, 31 for two-dimensional geometry and in Figs.32-34 for three-dimensional geometry. It is evident from these figures that statement of the problem under consideration corresponds to experimental data ERIM [2].

Two series of calculations have been executed. Emissivity of heated mixture of $\text{H}_2\text{O}/\text{N}_2$ was studied in the first series, and emissivity of heated mixture of CO_2/N_2 was studied in the second series.

The first series of calculations (mixture of $\text{H}_2\text{O}/\text{N}_2$)

In this case cylindrical volume of height $H_{hc} = 60$ cm contains mixture of water vapour and molecular nitrogen at temperature $T = 1202$ K and pressure $p = 0.1$ atm. Molar fractions of these species are: $x_{\text{H}_2\text{O}} = 0.5$, $x_{\text{N}_2} = 0.5$. These conditions correspond to experimental data [2] (Test-9R). Because at absence of radiation scattering a radius of heated cylinder does not effect on the emissivity. Therefore this value was assumed as $R_{hc} = 30$ cm. Numerical experiments with different values of R_{hc} are supported this assumption.

Numerical prediction of spectral radiation intensity of the heated volume in normal direction to plane surface, and corresponding experimental data [2] are shown in Fig.35. Optical properties of heated H_2O were borrowed from NASA standard infrared radiation model [3], where rotational line structure was averaged in each spectral group of $\Delta\omega = 25 \text{ cm}^{-1}$. Experimental data [2] are presented for spectral region $\Delta\Omega = 3000 \div 4200 \text{ cm}^{-1}$. Our calculations were performed with the same spectral resolution. Spectral absorption coefficient calculated at these conditions is shown in Fig.36.

Note, that the Problem IV actually identical to Problem I, because a non-scattering medium is considered. As it was shown above, calculation code Plume-2D-MC provides satisfactory accuracy of spectral radiation intensity prediction (about ~5%). Numerical simulation results obtained for Problem IV confirm this conclusion. It is easy to verify this, because the heated volume is homogeneous, and spectral radiation intensity can be calculated by relation (1) with the use of spectral values J_ω , $J_{b,\omega}$ and κ_ω . Therefore observed in Fig.35 good agreement between

theoretical prediction and ERIM experimental data indicates that optical model [3] provides adequate data.

Schematic of the problem for three-dimensional case is shown in Figs.32–34, and numerical simulation results for spectral intensity obtained by code Plume-3D-MC are shown in Fig.37. The NASA standard infrared radiation model of absorption coefficient averaged on rotational line structure was used in this case. Reference to Figs.35 and 37 shows that there is good enough agreement between numerical prediction and experimental data.

The second series of calculations (mixture of CO₂/N₂)

Cylindrical volume involving heated mixture of CO₂/N₂ at temperature $T=1200$ K and total pressure $p=0.1$ was considered in this case. Molar fraction of gas species are $x_{\text{CO}_2}=0.5$, $x_{\text{N}_2}=0.5$. Other initial conditions were the same as in the first calculation series.

Numerical simulation results for spectral intensity obtained with the use of code Plume-2D-MC are shown in Fig. 38. The NASA standard infrared radiation model [3] was used in these calculations. Averaged over rotational line structure spectral absorption coefficient of hot mixture CO₂/N₂ for conditions of experimental research [2] (Test 5) is shown in Fig.39.

Considered above numerical prediction of spectral radiation intensity of heated volumes of H₂O/N₂ and CO₂/N₂ for conditions of experiments [2] (Test 9R and Test 5), were obtained with the data accumulated in NASA standard infrared model [3]. It is of great practical interest to consider possibility to use other optical models for interpretation of the experimental data. Results of the investigation will be presented below.

Figure 40 shows spectral radiation intensity predicted by the use of narrow-band random model of rotational molecular lines [4] for conditions of Test-9R [2] (heated mixture of H₂O/N₂). As before, parameters of the random models were borrowed from database [3]. It is evident from the predictions presented in Figs.40 and 35 that the model of averaged line structure can be used in conditions under consideration for reasonable interpretation of experimental data [2].

Numerical simulation results for spectral radiation intensity at the same initial conditions, but with the use of HITRAN database [5], are shown in Fig.41. The model of averaged over rotational line structure spectral absorption coefficient, which is justified for optically thin layers, was used in the given case. The averaged in spectral region $\Delta\omega$ absorption coefficient was calculated for this case as follows:

$$\bar{\kappa}_{\Delta\omega_g} = \frac{1}{\Delta\omega_g} \sum_i^{N_g} S_i = \frac{1}{\Delta\omega_g} \int_0^{\Delta\omega_g} \sum_i^{N_g} \kappa_{\omega,i} d\omega, \quad (2)$$

where S_i is the intensity of the i -th rotational line (i.e., the integral absorption coefficient of the rotational line) inside the spectral region $\Delta\omega_g$; N_g is the total number of rotational line inside the spectral region $\Delta\omega_g$. Calculation code Plume-2D-MC uses for this case the following signs: $JLBL=0$, $JSUM=1$.

Figure 42 shows spectral radiation intensity predicted by another model of averaging. In this case the averaged spectral absorption coefficient was calculated as follows:

$$\bar{\kappa}_{\Delta\omega_g} = \frac{1}{\Delta\omega_g} \int_{\Delta\omega_g} \sum_i^{N_g} \kappa_{\omega,i} d\omega. \quad (3)$$

Spectral absorption coefficient of each rotational line $\kappa_{\omega,i}$ was calculated also with using HITRAN database. It is obviously, that due to very small value of half-width of each rotational line ($\gamma \sim 0.01 \text{ cm}^{-1}$) in conditions under consideration, formulas (2) and (3) should give close results. Observed differences in numerical predictions in Figs.41 and 42 are attributable to errors of numerical integration in Eq.(3), because only 2000 spectral points inside each spectral region $\Delta\omega_g$ was used.

Figure 43 shows spectral radiation prediction for the same conditions with the use of narrow-band random model of rotational lines [4] based on HITRAN database [5]. A comparison between data presented in Fig.43 and Fig.42 confirm our conclusion about possibility to use simple model of averaged rotational line structure in conditions under consideration.

Some optical models different from those listed above used also at interpretation of experimental data [2] for heated mixture CO_2/N_2 . We are reminding that numerical simulation results obtained with the use of optical model [3] are presented in Fig.38. Two spectral models based on HITRAN database [5] were used also for prediction of spectral radiation intensity for conditions of Test-5 [2]. Figure 44 shows results for averaging model (2) ($JLBL=0$, $JSUM=1$), and Fig.45 shows results for model (3) ($JLBL=0$, $JSUM=0$).

A narrow-band random model [4] based on rotational line parameters from database HITRAN [5] gives results shown in Fig.46 ($JLBL=3$).

A comparison between calculated data presented in Figs. 44–46 shows that all these models provide close results in conditions under consideration.

Spectral radiation intensity of heated mixture CO_2/N_2 (Test 5 [2]) was calculated also with the use of database CDSD-1000 [6], which is intended for prediction emission of CO_2 heated up to 1000 K. The numerical simulation results for the model of averaged rotational spectrum ($JLBL=0$, $JSUM=1$) and for narrow-band random model ($JLBL=3$) are presented in Figs. 47 and 48.

From the comparison of Figs.44–48 it appears that:

- a) Radiation heat transfer models realized in code Plume-2D-MC, which are based on databases of spectral optical properties of rotational lines HITRAN [5] and CDSD-1000 [6] allows predict spectral radiation intensity observed in experiments [2] with reasonable accuracy;
- b) Nevertheless, there is some significant discrepancy between calculation data based on HITRAN database and experimentally observed data in spectral regions $\Delta\omega=2100 \div 2250$ and $2400 \div 2450 \text{ cm}^{-1}$. Database CDSD-1000 provides better agreement between experimental and predicted data, but at $\omega > 2400 \text{ cm}^{-1}$ there is also significant discrepancy.

Analytical semi-empirical models [7, 8] were used also for interpretation of the ERIM experimental data. Numerical simulation results are shown in Figs.49 and 50. It is easy to verify that these models give reasonable agreement with the experimental data. It should be noted, that such kind of optical models very useful for methodical investigations of radiation heat transfer problems, but these models can not be recommended for precise calculations.

Let us consider also one peculiarity of numerical interpretation of experimental data. Figure 51,a shows temperature distribution in calculation domain which was used for calculations discussed above. If one will use temperature distribution, which is shown in Fig.51,b, it is possible to observe significant changes in spectral distributions of spectral intensity (see, for example, Figs.52 and 53). These differences are attributable to special features of radiation heat transfer through non-homogeneous gas layers with drastic variation of thermo-physical parameters.

Problem V.

Observation of spectral heat radiation of heated volume thought surrounding cold gas.

Interpretation of ERIM experimental data Test-9R (H₂O/N₂) and Test-5 (CO₂/N₂)

Schematic of the problem is shown in Fig.54 for the 2-dimensional formulation, and in Figs.55, 56 for the 3-dimensional formulation.

Initial conditions for the calculations were identical to real experimental investigation:

- Parameters of gas mixture inside heated volume:

$p = 0.1$ is the total pressure, atm,

$p_{\text{H}_2\text{O}} = 0.05$, $p_{\text{N}_2} = 0.05$ are the partial pressures of species, atm,

$H = 60$ is the height of the heated cylindrical volume, cm,

$T = 1202$ is the temperature of gas mixture, K;

- Parameters of surrounding cold gas:

$p = 0.07$ is the total pressure, atm,

$p_{\text{H}_2\text{O}} = 0.001$, $p_{\text{N}_2} = 0.069$ are the partial pressures of species, atm,

$L = 10\,000$ is the length of the optical path of observation, cm,

$T = 293$ is the temperature in surrounding gas, K.

Note, that parameters of hot gas model conditions in exhaust rocket plumes at altitude about ~16 km, and parameters of cold gas model optical path of ~28.8 km at altitude 18 km [2].

From the Figs.54-56 we notice that the calculation domain contains to sub-domains. The first one exactly corresponds to conditions of experiment Test-9R. The second one, which models volume of cold gas, is 100 times smaller than in real experimental situation. To model radiation transfer in real conditions, the following method is used in codes Plume-2D-MC and Plume-3D-MC. An effective pressure of H₂O in surrounding gas was introduced: $p_{\text{H}_2\text{O}}^* = 100 p_{\text{H}_2\text{O}} = 0.1$ atm, that is $x_{\text{H}_2\text{O}} = p_{\text{H}_2\text{O}}^* / p = 1.429$. But this effective pressure can be used only for prediction of averaged absorption coefficient (parameter S/d) for narrow-band random model of rotational lines. To calculate broadening of rotational lines in real surrounding conditions (parameter γ/d) one should use the real pressure $p = 0.07$ atm.

Prediction of hot-through-cold radiance with the use of models of averaged over rotational lines spectrum

Let us consider firstly numerical simulation results obtained by models of averaged over rotational line structure spectrum.

Prediction of hot cell and hot-through-cold spectral radiance by code Plume-3D-MC is shown in Figs.57,a. One can see from these data that essentially, the problem is as follows: a major portion of heat radiation is absorbed in surrounding gas, containing resonant absorbing cold gas.

Figure 57,b shows comparison of experimental data and numerical prediction of hot-through-cold spectral radiance for conditions of Test-9R experiments. Reference to Fig.57,b shows that maximal discrepancy between experimental data and numerical prediction fell within the region of maximal absorption ability of H₂O vibrational bands. At the same time, it is well known, that real spectra (vibrational bands) of emission and absorption contain large number of molecular rotational lines, therefore it might be assumed that the reason for the large discrepancy between experimental and numerical data is in using of non-adequate spectral optical model.

Figure 58 shows numerical predictions obtained by code Plume-2D-MC and optical model of averaged rotational structure of H₂O. Two upper curves correspond to radiance of hot cell, and two lower curves correspond to hot-through-cold radiance for different distances of observations (dotted line corresponds to 100 m, and solid line corresponds to 40 m).

First of all in should be noted good agreement of numerical simulation results provided by codes Plume-2D-MC and Plume-3D-MC. But, as before, there is large discrepancy between experimental and numerical data.

Numerical simulations presented above substantiate a necessity to use random models of rotational lines or more extensive line-by-line models, although both these kinds of models introduce new errors into numerical predictions.

Prediction of hot-through-cold radiance with the use of random models of rotational lines spectrum

Figures 59–62 show numerical prediction of hot-through-cold spectral radiance for ERIM experimental conditions Test-9R (mixture H₂O/N₂), obtained by code Plume-2D-MC with the use

of narrow-random models [4]. Numerical simulation data presented in Figs.59,60 correspond to NASA standard infrared radiation optical model [3], and data in Figs.61,62 were obtained with the use of parameters of rotational lines from HITRAN database [5].

The following two spectral optical models of radiation transfer were used for both databases:

- a) narrow-band random model for optically thin layers (Figs.59 and 61);
- b) narrow-band random model of real spectrum (Figs.60 and 62).

Numerical prediction of hot-through-cold spectral radiance for ERIM experimental conditions Test-5 (mixture CO₂/N₂), obtained by code Plume-2D-MC with the use of narrow-random models is shown in Figs.63.

With reference to presented numerical simulation data (Figs.60,62,63), it can be seen that narrow-band random models provide reasonable prediction of hot-through-cold spectral radiance for ERIM experimental conditions. From these numerical experiments some general conclusions can be also drawn regarding spectral optical models [3] and [5]: these models provide acceptable agreement of the numerical predictions.

However, some discrepancies between predicted and experimental data (inside separate spectral regions) have engaged our attention, and it substantiates necessity in further development of spectral optical models of heated gases and radiation heat transfer.

Prediction of hot-through-cold radiance with the use of line-by-line spectral models based on HITRAN-like databases

Figures 64,a-d show numerical prediction of hot cell spectral radiance for ERIM experimental conditions Test-9R (mixture H₂O/N₂), obtained by code Plume-2D-MC with the use of line-by-line model. These numerical simulation data were obtained with the use of parameters of rotational lines from HITRAN database [5].

Figure 64,a shows spectral intensity of hot cell radiance in spectral region $\Delta\Omega = 3000 \div 4400 \text{ cm}^{-1}$. This spectral region was divided by 56 spectral groups. The Monte-Carlo simulation of radiation transfer was performed in 3000 spectral points inside each spectral group. Thus, the spectral resolution of these calculations was about $\sim \Delta\omega = 0.0083 \text{ cm}^{-1}$. Figures 64,b-d

show the spectral intensity inside successfully decreasing spectral regions (up to $\Delta\Omega = 3450 \div 3452 \text{ cm}^{-1}$).

Figures 65,a-c show numerical prediction of hot-through-cold spectral radiance for ERIM experimental conditions Test-9R (mixture $\text{H}_2\text{O}/\text{N}_2$), obtained by code Plume-2D-MC with the use of line-by-line model. These numerical simulation data were also obtained with the use of parameters of rotational lines from HITRAN database [5].

With reference to Figs.64-65 it can be seen that the spectral intensity is changed inside range of ~ 5 orders. Therefore, it is easy to understand that the problem of averaging of the intensity in spectral region of $\sim \Delta\omega_g \sim 25 \text{ cm}^{-1}$ is very complex and difficult problem, which is very sensitive to many input factors of used models.

II.2. Test cases for code Plume-2D-MC

This part of the report contains list of test cases, which can be used for verification of the Plume-2D-MC code. Initial conditions for the test cases and graphical representation of numerical simulation results obtained in Radiative Gas Dynamic laboratory are presented in separate directories inside directory <Plume_MC_2D_Hybrid>.

Test Case 01

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of grey medium; $\kappa = 0.01$, $J_b = 1$. To execute this test case, one should change texts of the following two subroutines (see directory Plume_2D_MC_Hybrid/Calculation Test-01):

- SUBROUTINE GenCodeMC, lines 120–121;
- SUBROUTINE EXPELL, lines 183–186.

Number of simulating series and number of simulating photons inside the each series should be modified in file PARAM.dim.

Initial conditions for the test case are presented in directory Plume_2D_MC_Hybrid/Calculation Test-01/INPUT_Data

Exact value of the intensity must be as follows:

$$J = 1 \cdot (1 - e^{-0.0160}) = 0.451.$$

Graphical representation of results of the numerical simulations are presented in file
Plume_2D_MC_Hybrid/Calculation Test-01/RESULTS/Test-01_Intensity.wmf.

Test Case 02

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture H₂O/N₂ (“hot cell” radiance) at conditions of ERIM experiment (Test 9R).

The NASA standard infrared radiation model [3] is used.

Initial conditions for the test case are presented in directory
Plume_2D_MC_Hybrid/Calculation Test-02/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file
Plume_2D_MC_Hybrid/Calculation Test-02/RESULTS/Test-02_Intensity.wmf.

Test Case 03

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture H₂O/N₂ (“hot cell” radiance) at conditions of ERIM experiment (Test 9R).

The HITRAN database [5] is used for creation of averaged on rotational line structure optical model.

Initial conditions for the test case are presented in directory
Plume_2D_MC_Hybrid/Calculation Test-03/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file
Plume_2D_MC_Hybrid/Calculation Test-03/RESULTS/Test-03_Intensity.wmf.

Test Case 04

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture H₂O/N₂ (“hot cell” radiance) at conditions of ERIM experiment (Test 9R).

The semi-empirical analytical model [7] is used.

Initial conditions for the test case are presented in directory

Plume_2D_MC_Hybrid/Calculation Test-04/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file

Plume_2D_MC_Hybrid/Calculation Test-04/RESULTS/Test-04_Intensity.wmf.

Test Case 05

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture $\text{H}_2\text{O}/\text{N}_2$ (“hot cell” radiance) at conditions of ERIM experiment (Test 9R).

The semi-empirical analytical model [8] is used.

Initial conditions for the test case are presented in directory

Plume_2D_MC_Hybrid/Calculation Test-05/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file

Plume_2D_MC_Hybrid/Calculation Test-05/RESULTS/Test-05_Intensity.wmf.

Test Case 06

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture CO_2/N_2 (“hot cell” radiance) at conditions of ERIM experiment (Test 5).

The NASA standard infrared radiation model [3] is used.

Initial conditions for the test case are presented in directory

Plume_2D_MC_Hybrid/Calculation Test-06/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file

Plume_2D_MC_Hybrid/Calculation Test-06/RESULTS/Test-06_Intensity.wmf.

Test Case 07

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture CO_2/N_2 (“hot cell” radiance) at conditions of ERIM experiment (Test 5).

The HITRAN database [5] is used for creation of averaged on rotational structure optical model.

Initial conditions for the test case are presented in directory
Plume_2D_MC_Hybrid/Calculation Test-07/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file
Plume_2D_MC_Hybrid/Calculation Test-07/RESULTS/Test-07_Intensity.wmf.

Test Case 08

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture CO_2/N_2 (“hot cell” radiance) at conditions of ERIM experiment (Test 5).

The semi-empirical analytical model [7] is used.

Initial conditions for the test case are presented in directory
Plume_2D_MC_Hybrid/Calculation Test-08/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file
Plume_2D_MC_Hybrid/Calculation Test-08/RESULTS/Test-08_Intensity.wmf.

Test Case 09

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture CO_2/N_2 (“hot cell” radiance) at conditions of ERIM experiment (Test 5).

The semi-empirical analytical model [8] is used.

Initial conditions for the test case are presented in directory
Plume_2D_MC_Hybrid/Calculation Test-09/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file
Plume_2D_MC_Hybrid/Calculation Test-09/RESULTS/Test-09_Intensity.wmf.

Test Case 10

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture CO_2/N_2 (“hot cell” radiance) at conditions of ERIM experiment (Test 5).

The semi-empirical analytical model [8] is used.

This test case differs from Test Case 09 by the use of 60 spectral groups.

Initial conditions for the test case are presented in directory

Plume_2D_MC_Hybrid/Calculation Test-10/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file

Plume_2D_MC_Hybrid/Calculation Test-10/RESULTS/Test-10_Intensity.wmf.

Test Case 11

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture CO_2/N_2 (“hot cell” radiance) at conditions of ERIM experiment (Test 5). The CDSD-1000 database [6] is used for creation of averaged on rotational structure optical model.

Initial conditions for the test case are presented in directory

Plume_2D_MC_Hybrid/Calculation Test-11/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file

Plume_2D_MC_Hybrid/Calculation Test-11/RESULTS/Test-11_Intensity.wmf.

Attention: In this case one should change file HTR-HM.dim (see directory Plume_2D_MC_Hybrid/Calculation Test-11).

Test Case 12

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture $\text{H}_2\text{O}/\text{N}_2$ (“hot-through-cold” radiance) at conditions of ERIM experiment (Test 9R).

The NASA standard infrared radiation model [3] is used for calculation parameters of narrow-random model [4].

Initial conditions for the test case are presented in directory

Plume_2D_MC_Hybrid/Calculation Test-12/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file

Plume_2D_MC_Hybrid/Calculation Test-12/RESULTS/Test-12_Intensity.wmf.

Test Case 13

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture H_2O/N_2 (“**hot-through-cold**” radiance) at conditions of ERIM experiment (Test 9R).

The HITRAN database [5] is used for creation narrow-random model of rotational lines [4] ($JLBL = 2$).

Initial conditions for the test case are presented in directory Plume_2D_MC_Hybrid/Calculation Test-13/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file Plume_2D_MC_Hybrid/Calculation Test-13/RESULTS/Test-13_Intensity.wmf.

Test Case 14

Calculation of spectral radiation intensity in the normal direction to front plane surface of homogeneous cylindrical volume of heated mixture H_2O/N_2 (“**hot-through-cold**” radiance) at conditions of ERIM experiment (Test 9R).

The HITRAN database [5] is used for line-by-line calculation.

Initial conditions for the test case are presented in directory Plume_2D_MC_Hybrid/Calculation Test-14/INPUT_Data

Graphical representation of results of the numerical simulations are presented in file Plume_2D_MC_Hybrid/Calculation Test-14/RESULTS/Test-14_Intensity.wmf.

II.3. How to include new spectral optical models into the code Plume-2D-MC

1. Instead of the following operator in SUBROUTINE GenCodeMC (lines 108-112)

```
CALL OPTICS(TGAS,OMEGS,PRESIJ,AGL,OMIS,OMAS,
,          JOptModel,JLBL,JSUMS,JFIRST,
,          AB_H2O,AB_CO2,AB_CO,AB_NO,AB_HCL,AB_HF,
,          DL_H2O,DL_CO2,DL_CO,DL_NO,DL_HCL,DL_HF,
,          DD_H2O,DD_CO2,DD_CO,DD_NO,DD_HCL,DD_HF)
```

one should use the following operator in SUBROUTINE GenCodeMC (lines 113-117)

```
CALL New_OPTIC_Model(TGAS,OMEGS,PRESIJ,AGL,OMIS,OMAS,
,          JOptModel,JLBL,JSUMS,JFIRST,
```

```
,      AB_H2O,AB_CO2,AB_CO,AB_NO,AB_HCL,AB_HF,
,      DL_H2O,DL_CO2,DL_CO,DL_NO,DL_HCL,DL_HF,
,      DD_H2O,DD_CO2,DD_CO,DD_NO,DD_HCL,DD_HF)
```

2. It is necessary to fill out empty SUBROUTINE New_OPTICS_Model, which is located in file OPTICS.FOR (lines 1039-1111). All necessary comments are presented inside the subroutine. If one will add any own code for line-by-line calculations, it is necessary to input JLBL=1 in initial data (INPUT_Data/INPUT_MC_Plumes.DD).

III. Conclusion

1. It has been shown that spectral signature and spectral intensity of heat radiation of heated volumes can be predicted by code Plume-2D-MC with accuracy about 5% at number of simulating photons of 10^5 for each spectral group.

2. Investigation of computational convergence of statistical simulation results versus number of simulating photons has been performed and corresponding results have been presented in the report.

3. Verification of code Plume-2D-MC has been performed by comparison of numerical simulation results with exact analytical solutions and with numerical simulation results predicted by code Plume-3D-MC.

4. Verification of code Plume-2D-MC has been executed on the examples of radiation heat transfer in volumes of different geometries (infinite plane layer, spherical and cylindrical volumes).

5. Numerical simulation prediction of ERIM experimental data for hot cell radiance has been performed. It has been shown that NASA standard infrared optical model [3] provides good agreement between experimental data (Test 9R и Test 5 [2]) and numerical predictions for H_2O (band $27\ \mu$) and satisfactory agreement for CO_2 (band $4.3\ \mu$).

6. Influence of different optical models on predicted numerical data on hot cell radiance for ERIM experimental conditions has been studied.

7. Numerical simulation prediction of ERIM experimental data for hot-through-cold radiance has been performed. It has been shown that using spectral optical models of averaged over rotational line structure spectra leads to large errors of the predictions. It does not depend on used spectral optical models (NASA standard infrared radiation model [3] or HITRAN database [5]).

8. It has been shown that using narrow-band random models, taking into account rotational line structure of spectra, for prediction of hot-through-cold radiance provide good enough agreement between experimental and numerical data. It does not depend on used spectral optical models (NASA standard infrared radiation model [3] or HITRAN database [5]). However, some discrepancies between predicted and experimental data (inside separate spectral regions)

have engaged our attention, and it substantiates necessity in further development of spectral optical models of heated gases and radiation heat transfer.

9. Numerical simulation prediction of ERIM experimental data for hot cell radiance with the use of the line-by-line calculations has been performed. It has been shown that HITRAN-like databases can be used together with calculation code Plume-2D-MC for prediction of spectral signature with high spectral resolution.

10. Description of 14 calculation test cases has been presented.

11. Technical documentation for using code Plume-2D-MC has been presented.

12. Source texts of the code Plume-2D-MC has been presented with necessary commentaries.

IV. References

1. Kotov D.V., Surzhikov S.T. “Benchmark Solutions for the Monte-Carlo Simulation Prediction of Spectral Signatures”, AIAA 05-4947, 2005, 11 p.
2. Lindquist G.H., Arnold C.B., Spellicy R.L. Atmospheric Absorption Applied to Plume Emission. Experimental and Analytical Investigations of Hot Gas Emission Attenuated by Cold Gases. Report ERIM No. 102700-20-F, AFRPL-TR-75-30. August 1975, 208 p.
3. Ludwig C.B., Malkmus W., Reardon J.E., Thomson J.A.L. Handbook Infrared Radiation from Combustion Gases. Scientific and Technical Information Office. National Aeronautics and Space Administration, Washington, D.C., 1973.
4. Surzhikov S.T., Howell J.R. “Monte-Carlo Simulation of Radiation in Scattering Volumes with Line Structure”, J. of Thermophysics and Heat Transfer, 1998, Vol. 12, No. 2, pp. 278–281.
5. Rothman L.S., Gamache R.R., Tipping .H., et al., «The HITRAN Molecular Database: Editions of 1991 and 1992,» JQSRT, 1992, Vol.48, No.5/6, pp.469–518; Also edition of 1996 (on CD).
6. Tashkun S.A., Perevalov V.I., Teffo J.-L., et al. CDSD-1000, The high temperature carbon dioxide spectroscopic databank. JQSRT, 2003, Vol. 82, pp.165–196
7. Surzhikov S.T. Optical Properties of Gases and Plasmas. Moscow, Moscow State Technical University Press, 2004, 575 p. (in Russian)
8. Li W., Tong T.W., Dobranich D., Gritz L.A. “A Combined Narrow- and Wide-Band Model for Computing the Spectral Absorption Coefficient of CO₂, CO, H₂O, CH₄, C₂H₂, and NO”, JQSRT, 1995, Vol. 54, No. 6, pp.961–970.

V. List of published papers

1. Surzhikov, S.T., "Direct Simulation Monte-Carlo Algorithms for the Rocket Exhaust Plumes Emissivity Prediction," AIAA Paper 2002-0795, 40th Aerospace Sciences Meeting & Exhibit, 2002, Reno, NV. P.11

The basic idea of a band model is simply to spread the integrated line strength of a given transition over the frequency interval defined by nearest neighbor lines. This limits the ultimate resolution of a band model to the local line spacing which is less than $\sim 1 \text{ cm}^{-1}$. Near a band-head the line spacing decreases greatly and it is even possible to apply band models in this spectral region to below $\sim 0.1 \text{ cm}^{-1}$. The approximations introduced into this band-model formulation were made with the ultimate resolution in mind. That is, terms were omitted which would shift line locations or spacing by approximately 0.1 cm^{-1} or less.

Some methods of numerical simulation of spectral, multi-group, and total characteristics of radiation heat transfer in SRM exhaust plumes are considered.

The first group includes calculation methods allowing obtain an accurate solution of the radiation heat transfer equation [1]. The area of problems accepting the accurate solution is extremely narrow. Besides that there are strict limits applied to the examined region geometry, medium optic properties, and boundary conditions.

The second group includes approximate deterministic methods of the radiation heat transfer equation solution, for example, the Spherical Harmonic method, the Discrete Ordinates method (DOM), the Discrete Direction Method (DDM), etc. [2,3].

The third group consists of statistical solution methods of the radiation heat transfer equation. This group includes in one's turn the Direct Simulation Monte-Carlo methods (DSMC) [2,4-9], and statistical solution methods of the radiation heat transfer equation in the integral form.

This paper presents some traditional and novel algorithms of DSMC methods which are widely applied for solving of actual radiation heat transfer (RHT) problems. Inasmuch as the term "DSMC" is usually used for problems of rarefied aerodynamics, the term "RHT/DSMC" will be used below.

The computational algorithm detail description is presented. Alternatively methods and the truth estimation methods of the simulating results are discussed. Numerical simulation results are presented for the problem of prediction of the directional multigroup emissivity of rocket exhaust plumes [10-14].

2. Surzhikov, S.T., "Spectral and Narrow Band Directional Emissivity of Light-Scattering and Non-Scattering Volumes," AIAA Paper 2002-3324, 8th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, June 2002, St. Louis, Missouri. p.11.

A comparison of various models of spectral optical properties of heated gases CO_2 and H_2O , intended for use in calculations of directional emissivity of light-scattering and non-scattering volumes is presented. The following models are analyzed:

a) The NASA infrared radiation model (Ludwig, C.B., Malkmus, W., Reardon, J.E., Thomson, J.A.L., Handbook Infrared Radiation from Combustion Gases. NASA, Washington, D.C., 1973); b) An averaged absorption coefficients based on the temperature-extrapolated HITRAN data; c) An averaged absorption coefficients based on theoretical prediction (Khmelinin, B.A., Plastinin, Yu.A., TSAGi Transactions No.1656, 1975 (in Russian)); d) The Edwards wide-band models; e) An improved wide-band models.

The Half-Moment method for solving of radiation heat transfer problems in non-homogeneous plane layers of heated gases is developed. The temperature-extrapolated data from the HITRAN database are used for the line-by-line calculations and for creation of random models. Distributions of radiation heat fluxes calculated by the line-by-line and random models are compared.

A Direct Simulation Monte-Carlo method is used for prediction of monochromatic signature of a model solid rocket motor (MSRM), investigated by H.F. Nelson (J. of Spacecraft and Rockets, 1987, Vol.24, No.6).

Calculations of rocket exhaust signatures were performed for different optical models investigated in the first part of the paper.

3. Surzhikov, S.T., Levine, J., “Time-Dependent Spectral Radiation of Fire Ball Generated at Rocket Explosion,” AIAA Paper 2003-1054, 41st Aerospace Sciences Meeting & Exhibit, 2003, Reno, NV. P11

A statement of the problem and numerical simulation data on spectral radiation emission of a fireball generated at rocket explosion at active part of a trajectory is presented. Prediction of gasdynamics of the fireball is based on the Reynolds averaged Navier–Stokes equations united in self-congruent system of equations of continuity for chemical species, equations for transfer of energy of turbulent pulsation, and radiation heat transfer equation. Two methods are used for solving radiation heat transfer equation. The first one is the Spherical Harmonic method. This method is used for calculation of radiative energy balance in the fireball during its moving in free atmosphere. The second one is the Monte-Carlo simulation of radiation heat transfer, which is used for prediction of spectral directional emissivity of the fireball.

The ultimate aim of this consideration is prediction of the fireball spectral signature time dependence. The unsteady signature of a fireball is calculated for its typical lifetime ~20 s.

4. Surzhikov, S.T. “Monte-Carlo Simulation of Plumes Spectral Emission,” AIAA Paper 2003-3895, 36th AIAA Thermophysics Conference, 23-26 June 2003, Orlando, Florida, pp.1–11.

Monte Carlo simulation algorithms, intended for calculation of spectral directional emissivity (spectral signature) of solid rocket motor (SRM) plumes on non-orthogonal grids are submitted.

Comparative analysis of three imitating algorithms is given: the two line-by-line methods of Monte-Carlo simulation united with algorithms of the Maximal Cross-Section (MCS) and quasi-random sampling (QRS) of parameters of photon trajectories, and also the hybrid simulation method based on statistical models of molecular rotational lines.

5. Surzhikov, S.T. “Prediction of 3D Rocket Exhaust Plume Signatures by the Monte-Carlo Method,” AIAA Paper No.04-1354, 2004, 42nd Aerospace Sciences Meeting & Exhibit, Reno, NV, pp.1–11.

Computing model for numerical simulation of the three dimensional spectral signatures of rocket exhaust plumes by the Imitating Monte-Carlo method are presented. The model includes proper of the imitating Monte-Carlo algorithms and is consisted with spectral methods for interpretation of molecular lines fine structure of emitting spectra.

Numerical simulation results for sunlight scattering on high-altitude space vehicle plume and for three-dimensional plume of heavy launch vehicle are presented.

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Analysis of possible radiation heat transfer problems which can be considered as the test cases, and description of a new Monte-Carlo simulation algorithm (the Monte-Carlo Local Estimation of Directional Emissivity – MCLEDE) for prediction of spectral signatures of one-, two- and three-dimensional light-

scattering volumes are presented. Suggested method can be recommended both for generation of benchmark solutions and for practical use in different aerospace applications.

7. Surzhikov S.T. “Hybrid Monte-Carlo/Random Model of Molecular Lines Algorithms for Signature Prediction,” AIAA 06-1187. 2006. 44th Aerospace Sciences Meeting & Exhibit, Reno, NV. 18 p.

The paper presents description of numerical study of computing code Plume-2D-MC. This computing code is intended for prediction of spectral directional emissivity (spectral signature) of heated gas volumes, and for prediction of an attenuation of the heat radiation by long paths of cold atmospheric gases. Code Plume-2D-MC realizes several Monte-Carlo simulation algorithms, and several spectral optical models of heated gases (the NASA standard infrared model, the HITRAN database, the CSDS-1000 database, some analytical semi-empirical wide-band models, and analytical semi-empirical wide/narrow models). The paper presents results of study of mathematical accuracy of imitating Monte-Carlo algorithms, which are used in the code Plume-2D-MC. The paper contains results of numerical predictions of ERIM experimental data of hot gas cells radiance, both unattenuated and attenuated by long atmospheric paths.

VI. List of presentations at conferences and meetings

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Appendix 1

Numerical simulation results

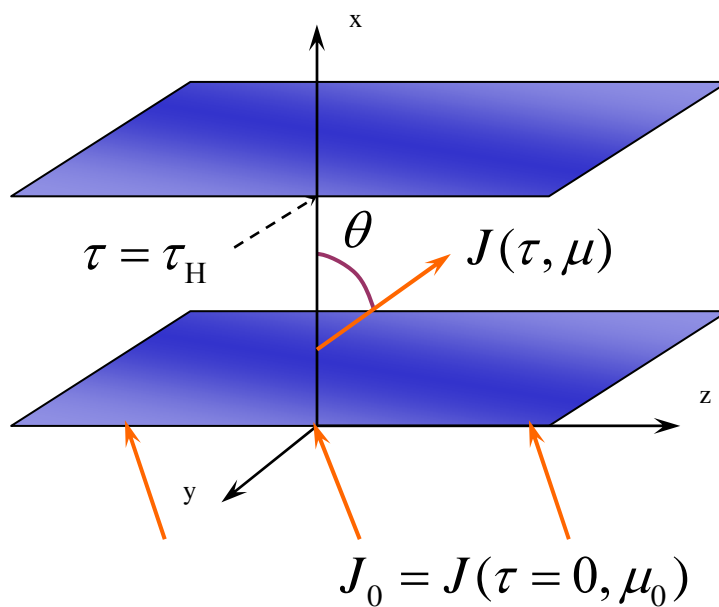


Fig. 1. Schematic of the Problem I:
Spectral intensity of heat radiation of plane layer in normal direction ($\theta=0$, $J_0=0$)

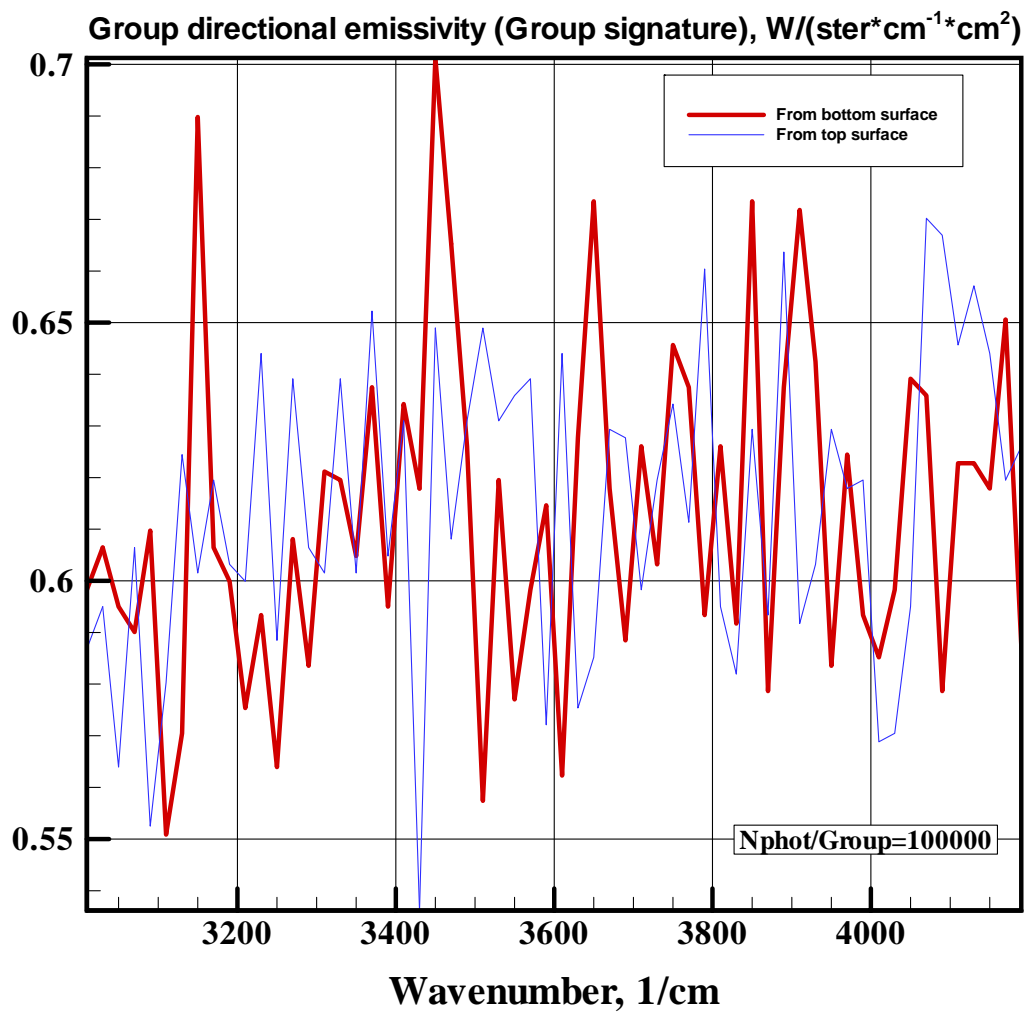


Fig.2. Problem I: Code Plume-2D-MC, $N_{ph} = 10^5$, $N_\theta = 21$

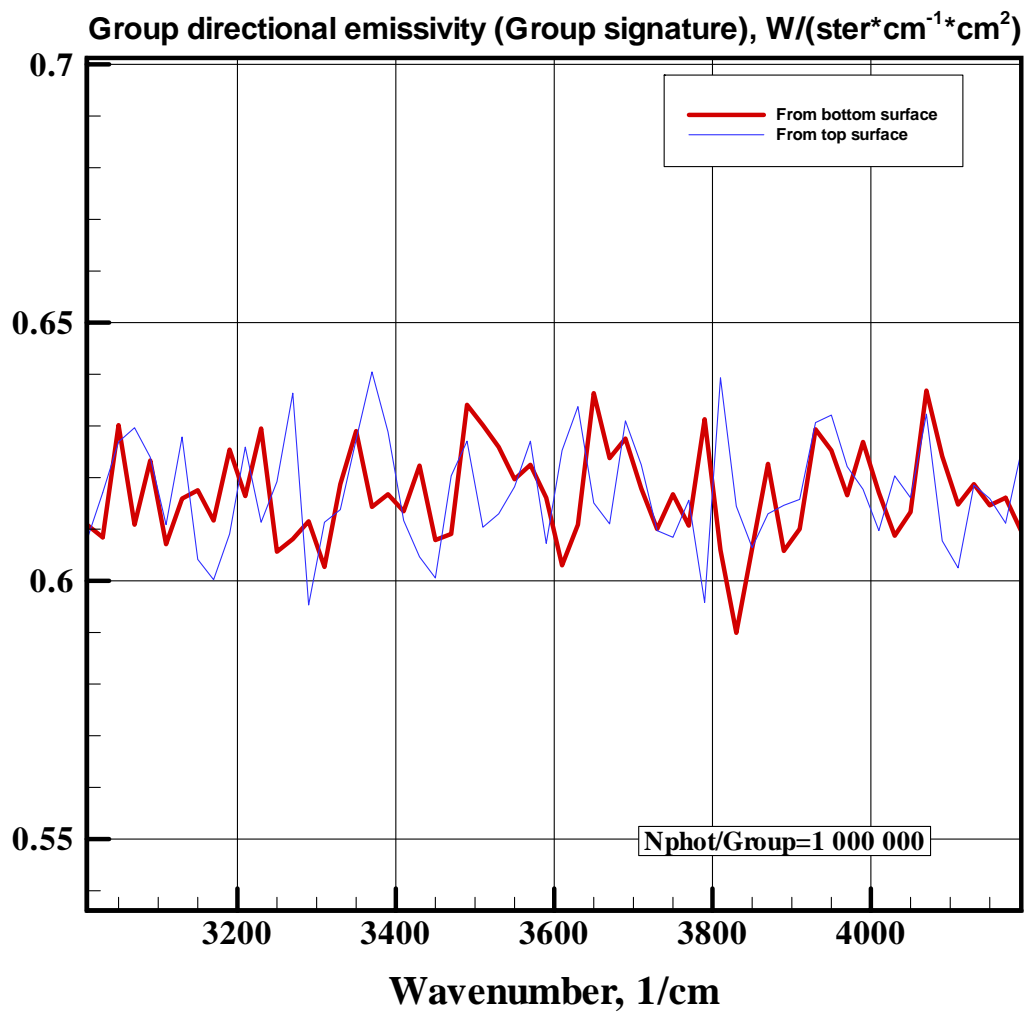


Fig.3. Problem I: Code Plume-2D-MC, $N_{ph} = 10^6$, $N_\theta = 21$

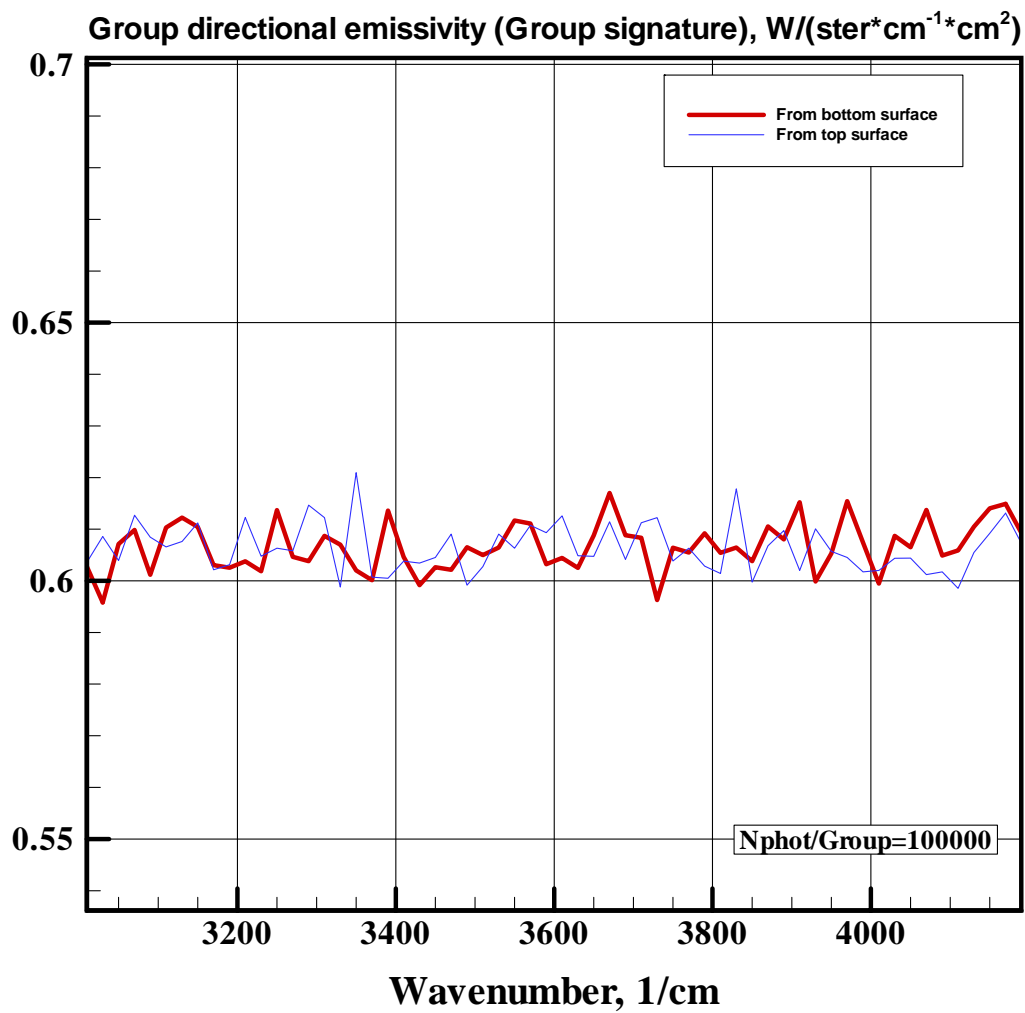


Fig. 4. Problem I: Code Plume-2D-MC, $N_{ph}=10^6$, $N_\theta=11$

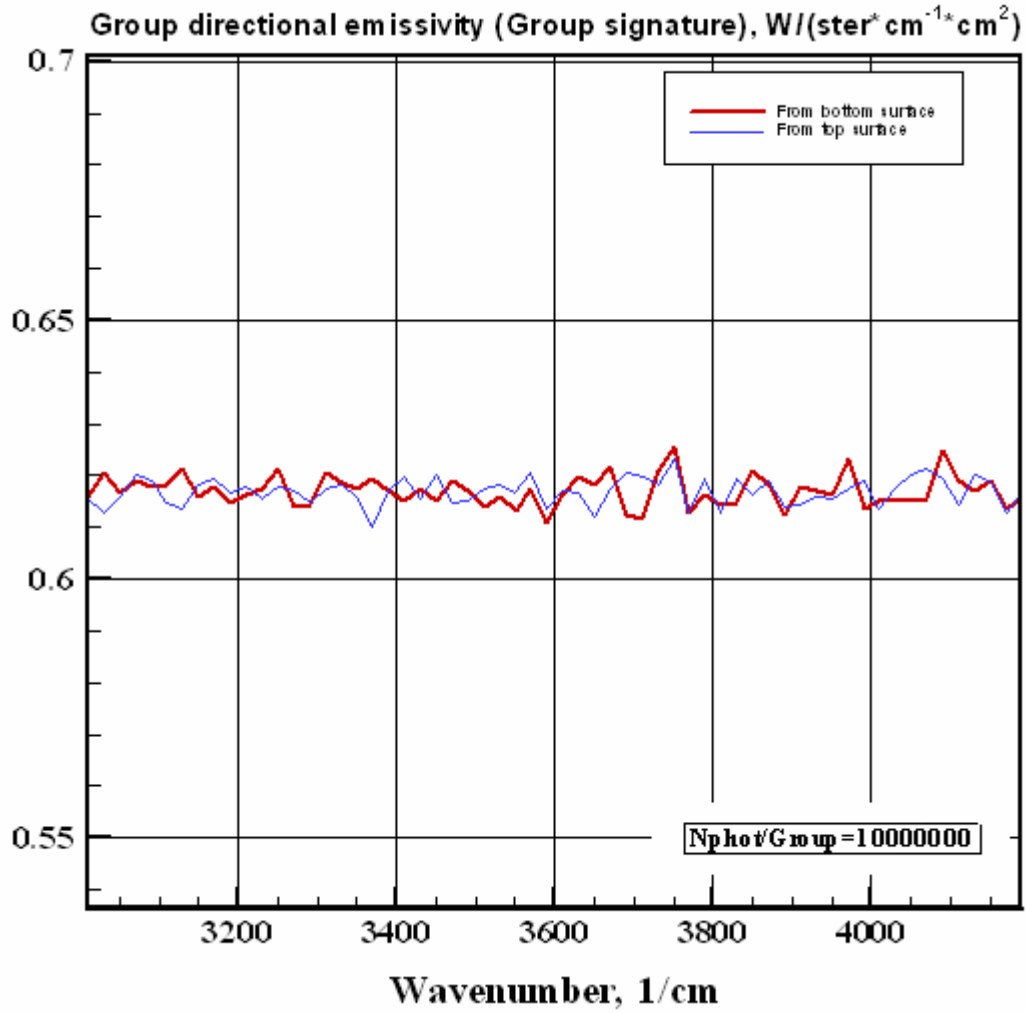


Fig. 5. Problem I: Code Plume-2D-MC, $N_{ph} = 10^7$, $N_{\theta} = 21$

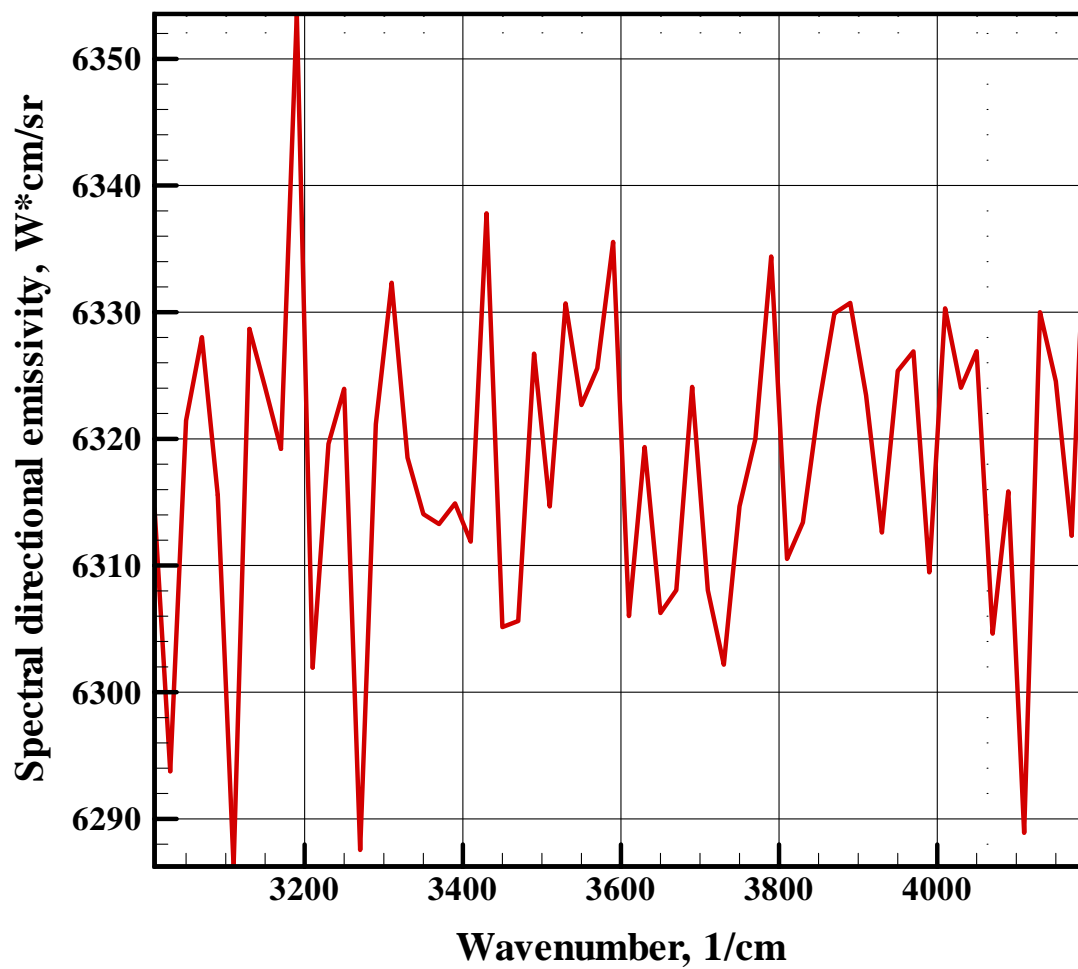


Fig. 6. Problem I: Code Plume-3D-MC, $N_{ph} = 5000$; algorithm **MCLEDE**

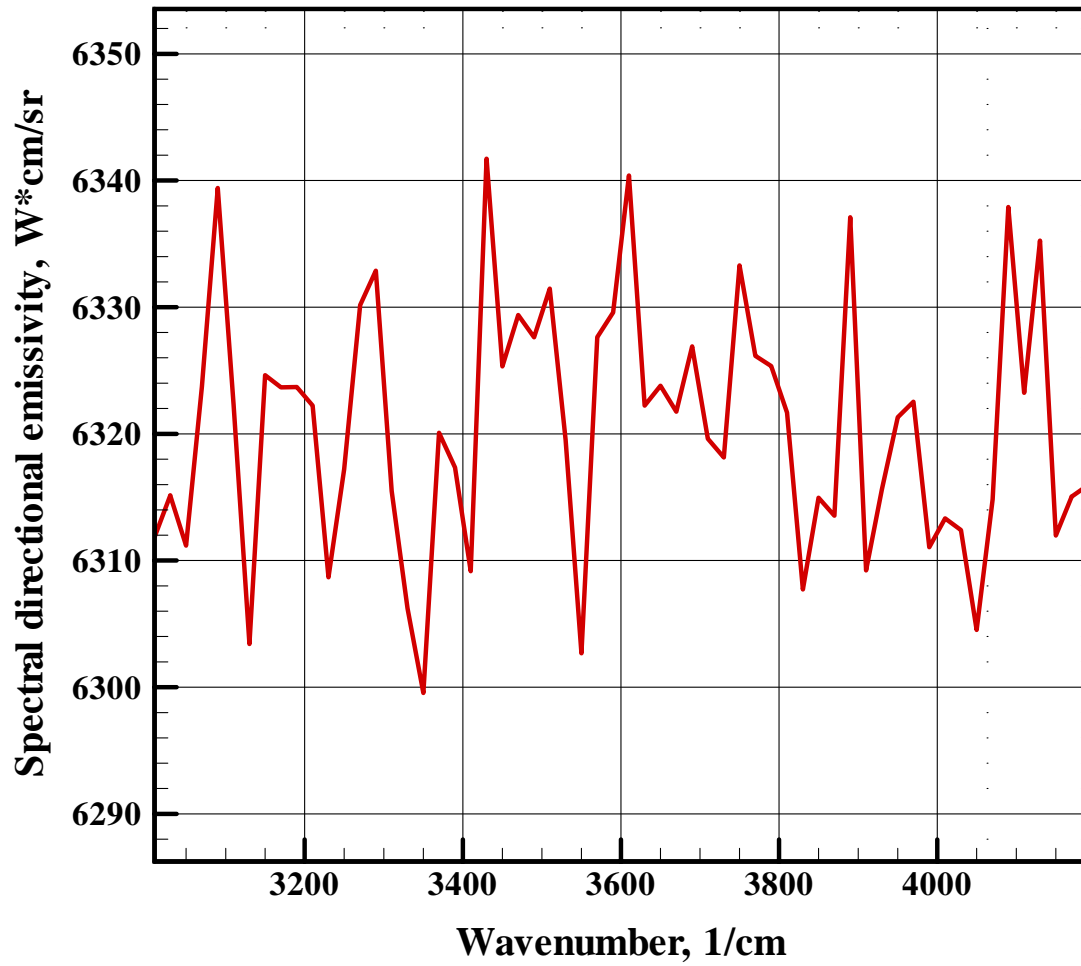


Fig. 7. Problem I: Code Plume-3D-MC, $N_{ph}=10^4$; algorithm **MCLEDE**

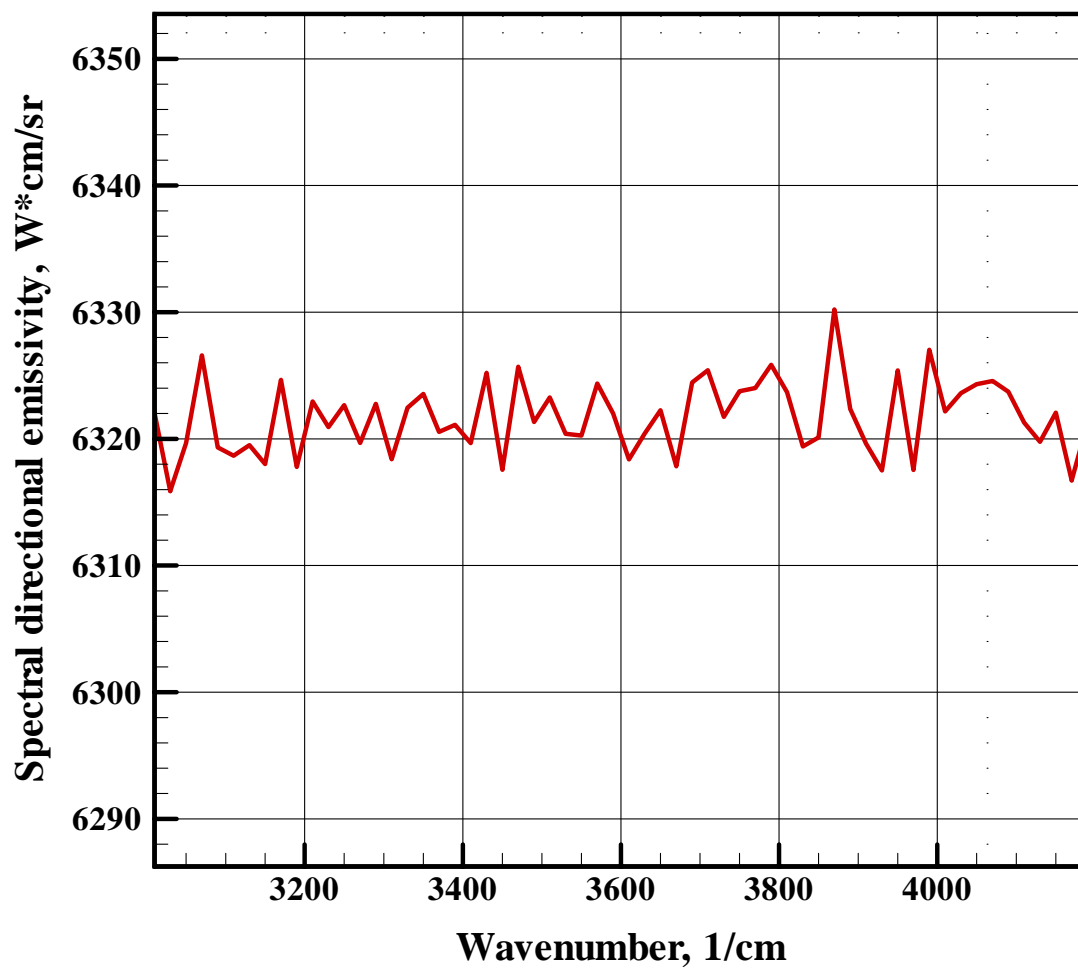


Fig. 8. Problem I: Code Plume-3D-MC, $N_{ph}=10^5$; algorithm **MCLEDE**

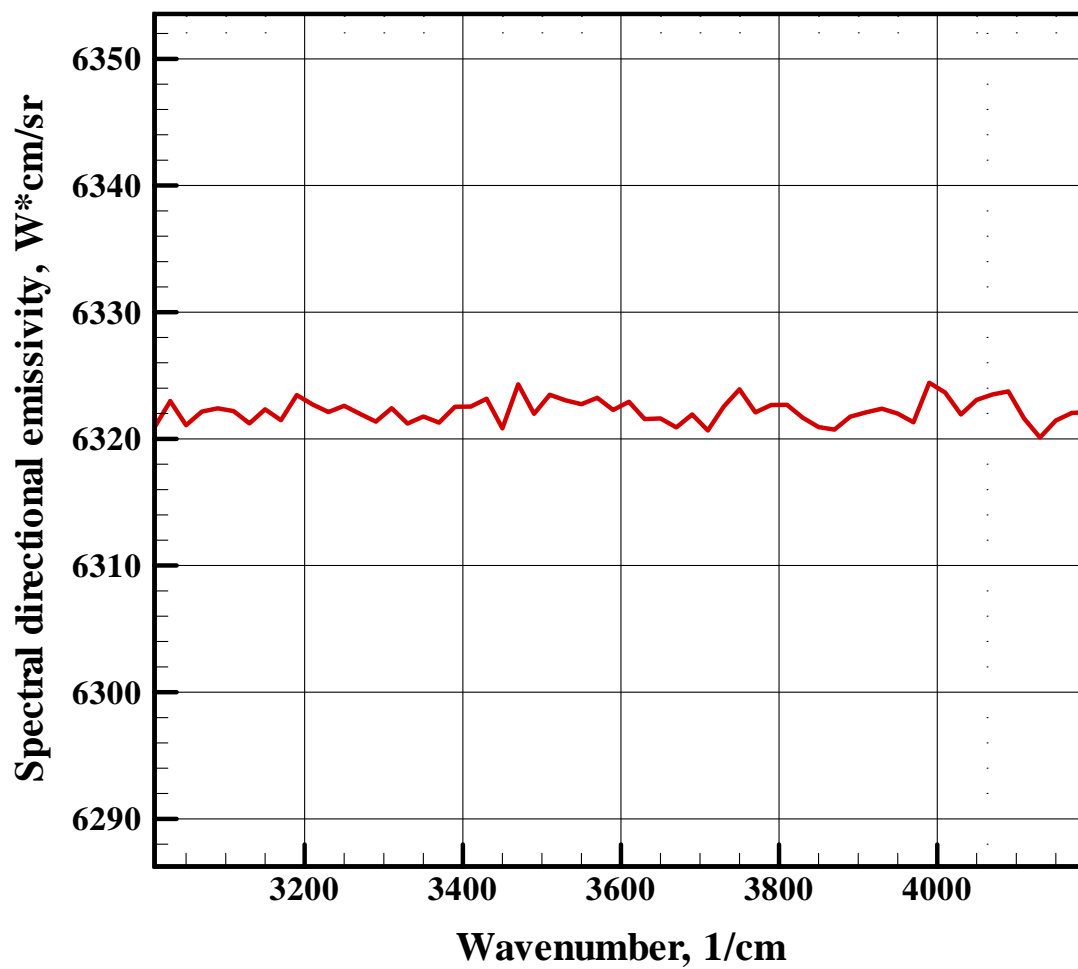


Fig. 9. Problem I: Code Plume-3D-MC, $N_{ph}=10^6$; algorithm **MCLEDE**

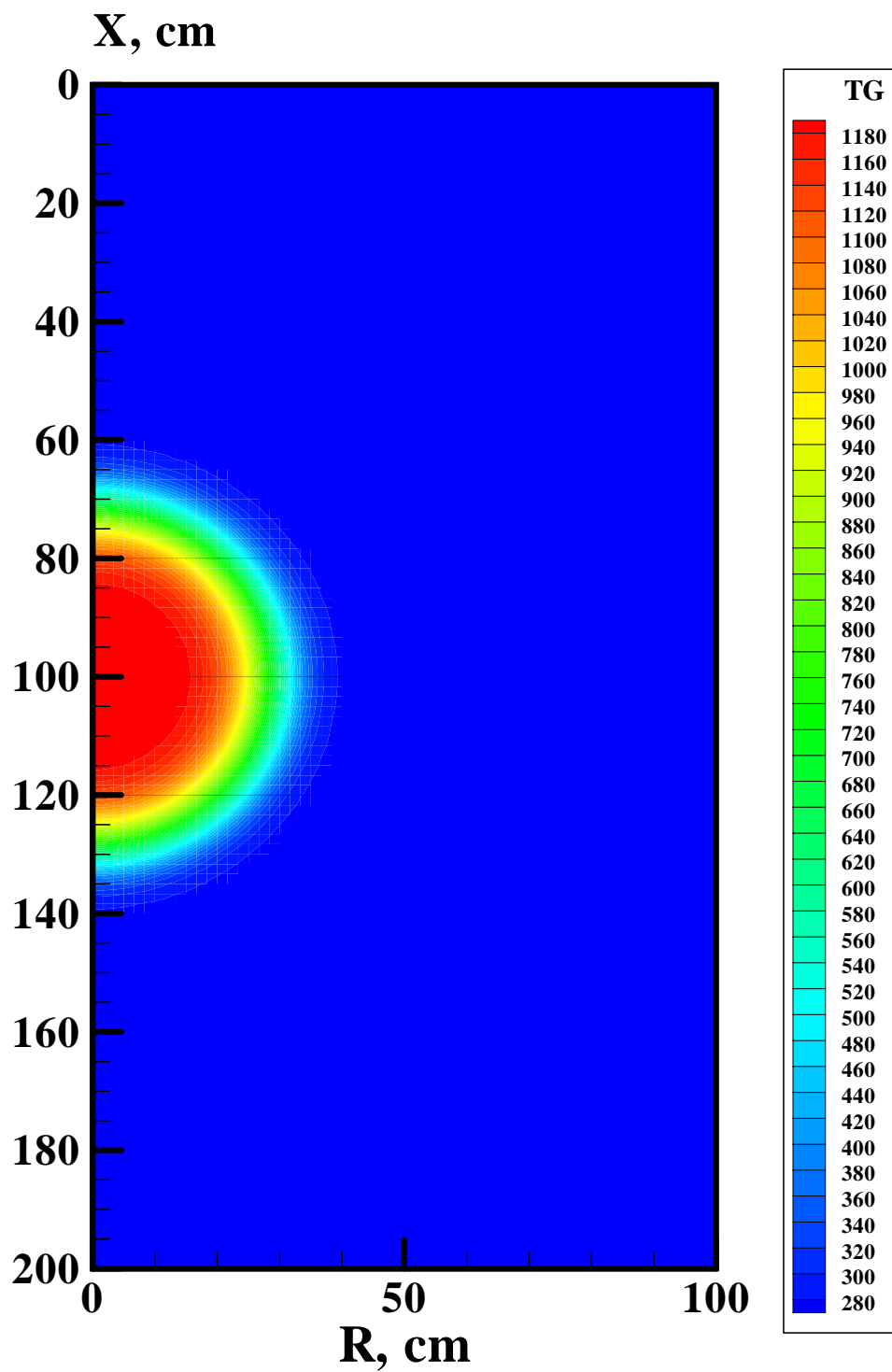


Fig.10. Problem II: Temperature field of spherical form in axisymmetric cylindrical geometry

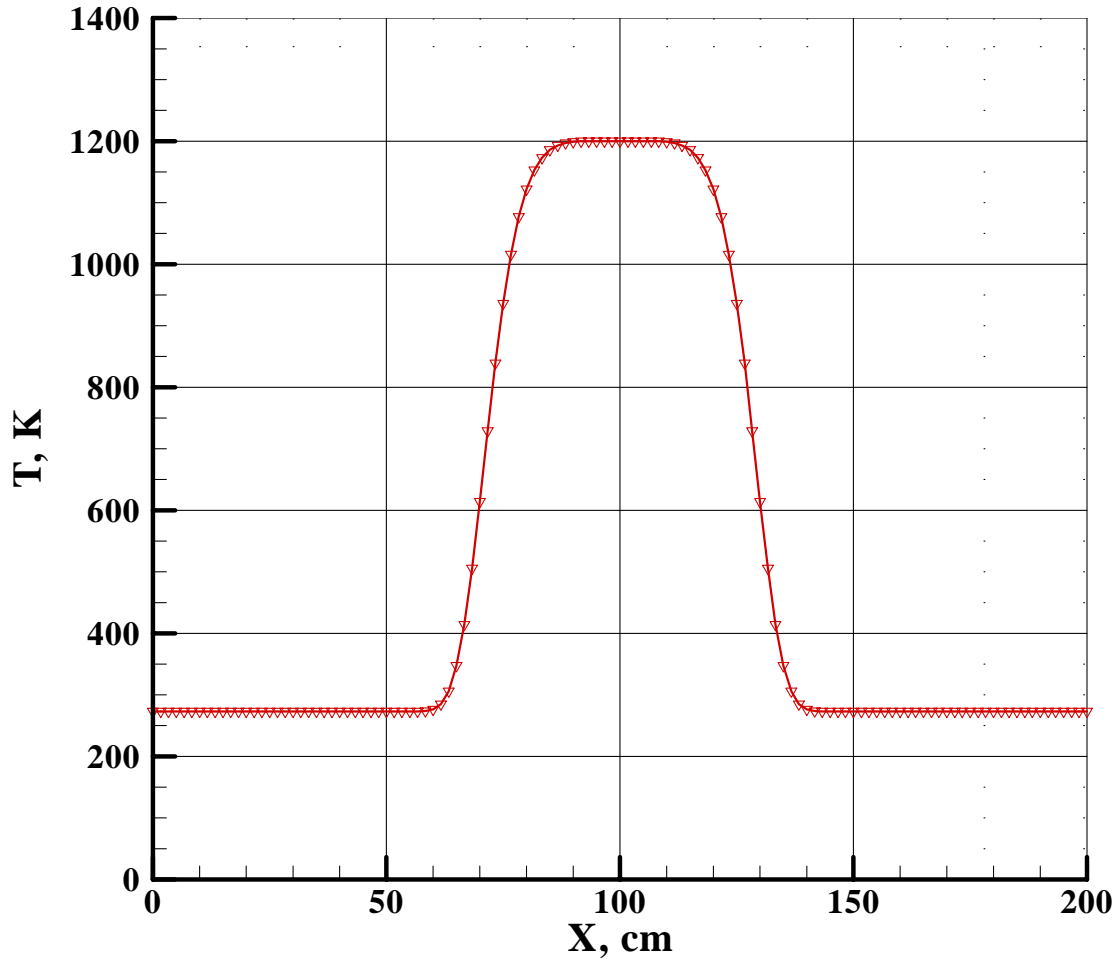


Fig.11. Problem II: Temperature distribution along axis of symmetry of cylindrical volume

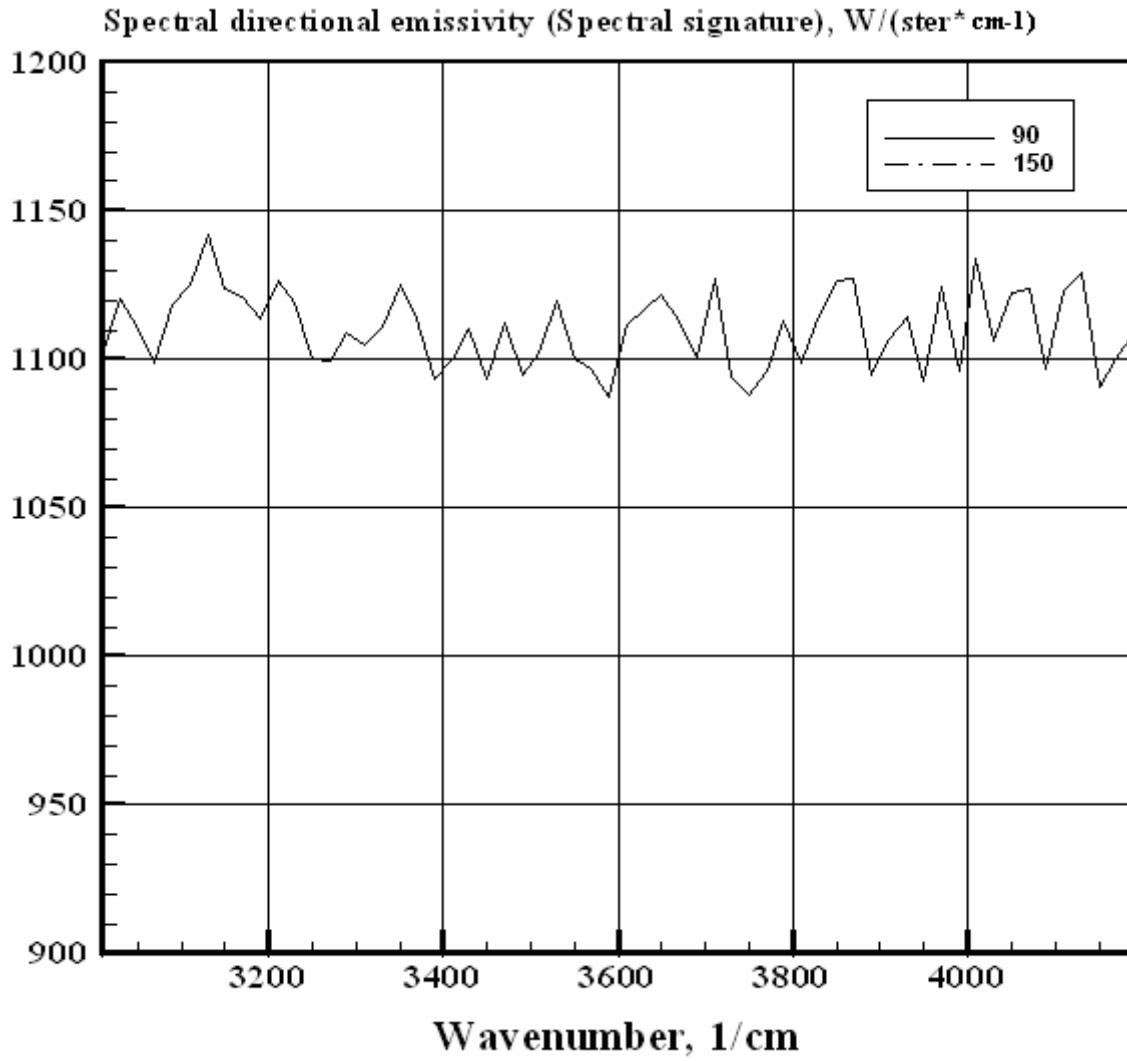


Fig. 12. Problem II: Spectral signature of homogeneous spherical volume from the cylindrical surface, $N_{ph}=10^5$

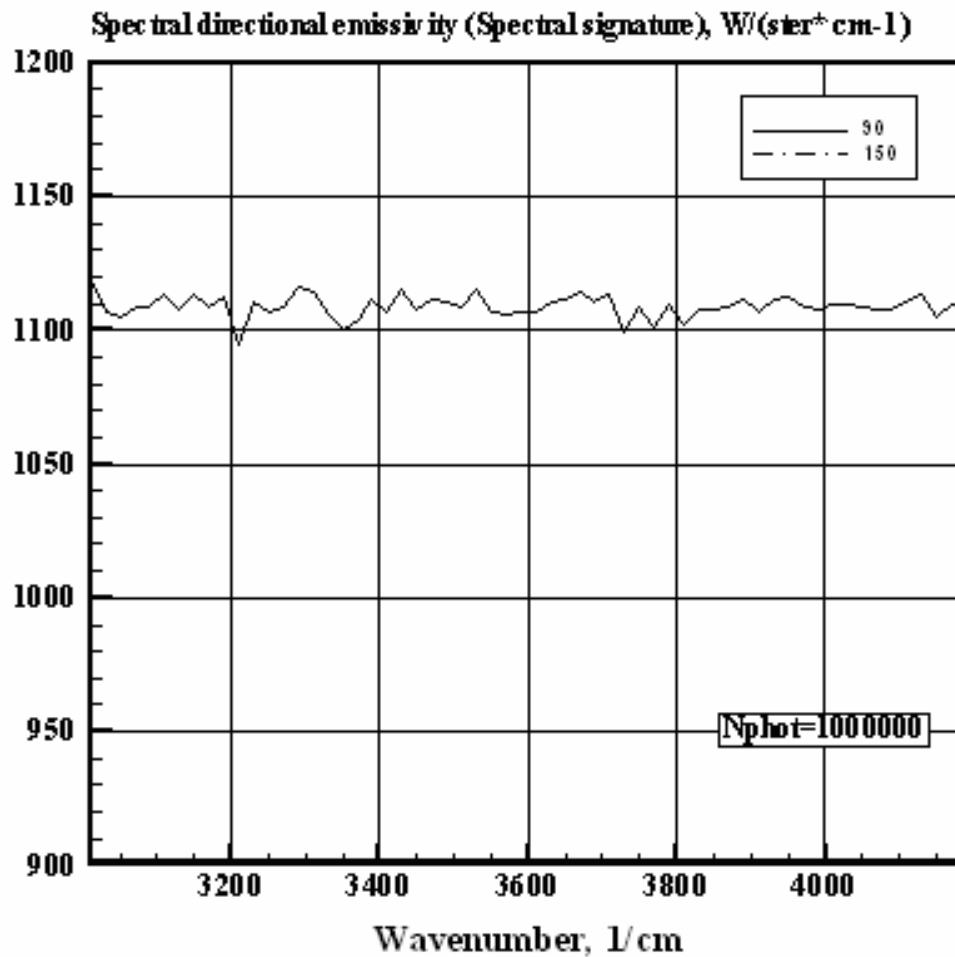


Fig. 13. Problem II: Spectral signature of homogeneous spherical volume from the cylindrical surface, $N_{ph}=10^6$

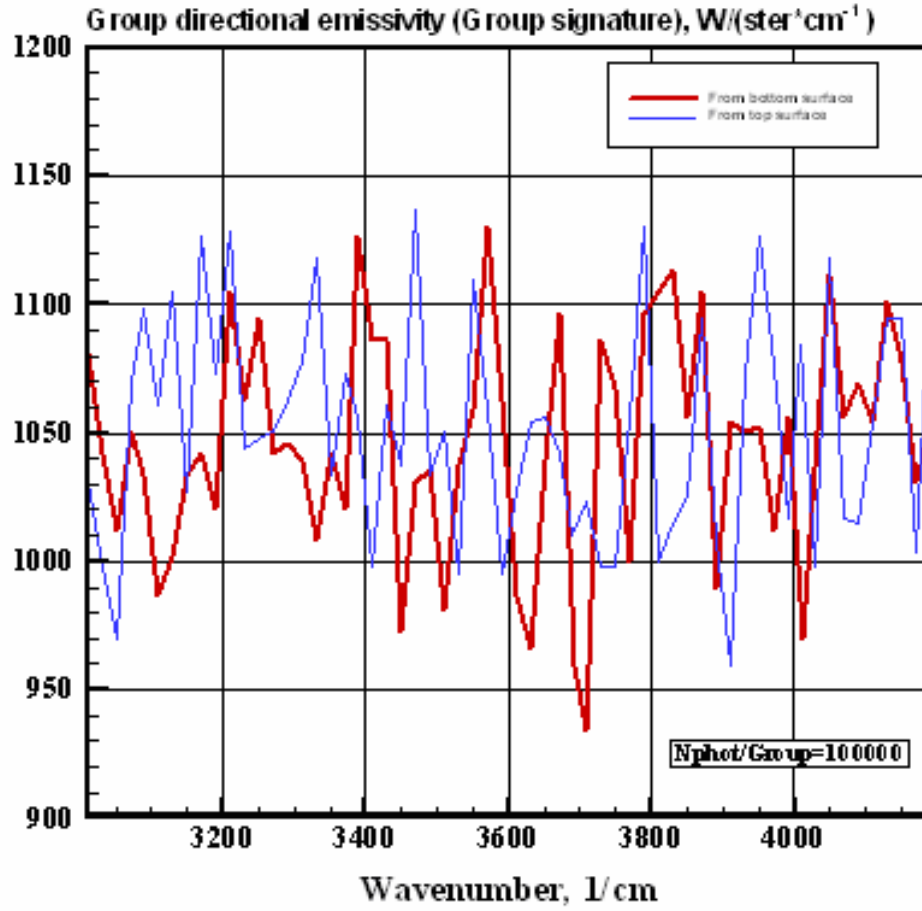


Fig. 14. Problem II: Spectral signature of homogeneous spherical volume from plane surfaces, $N_{ph}=10^5$

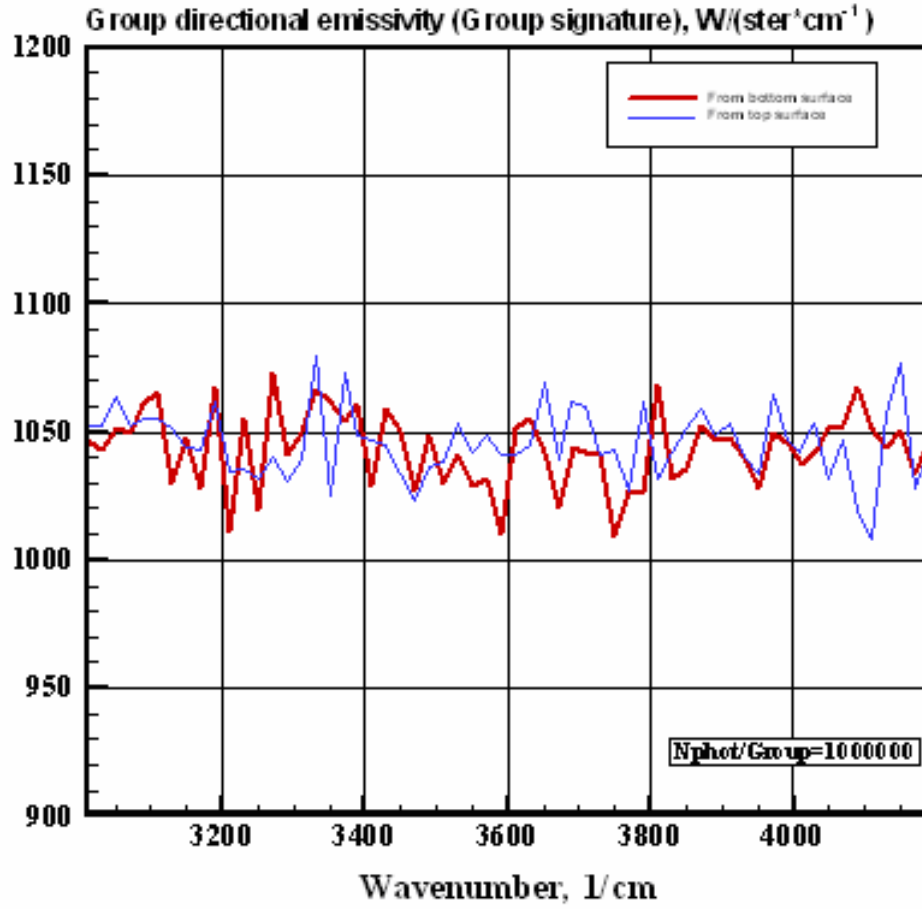


Fig. 15. Problem II: Spectral signature of homogeneous spherical volume from plane surfaces, $N_{ph}=10^6$

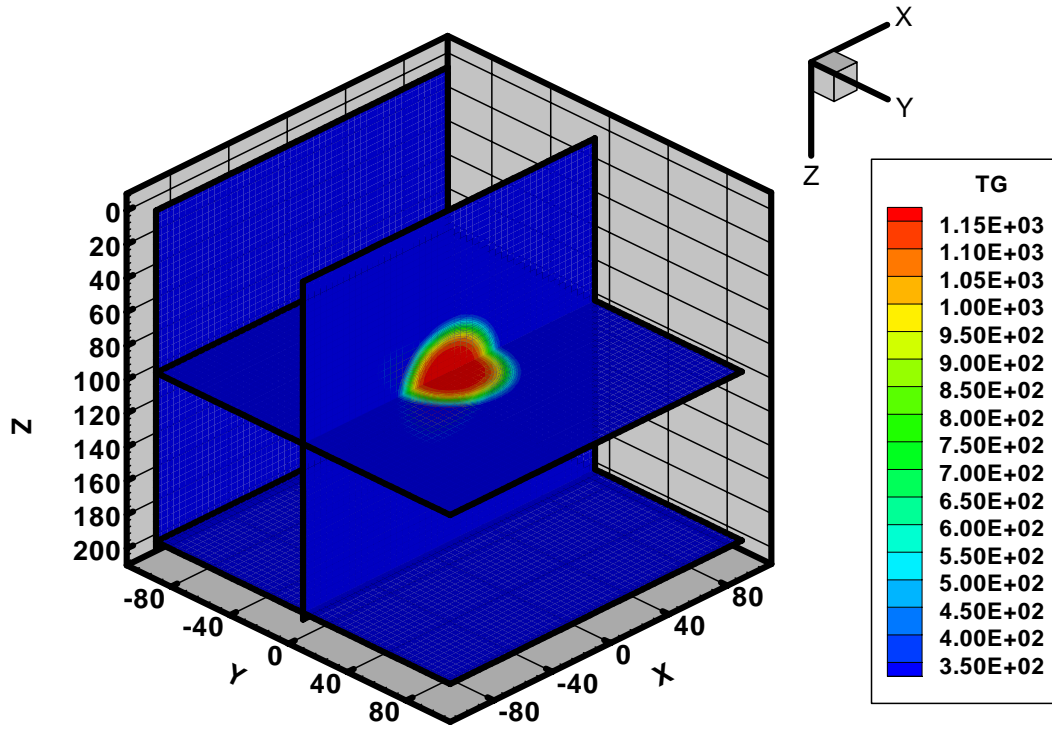


Fig.16. Problem II: Temperature field of spherical form in 3D Cartesian coordinates

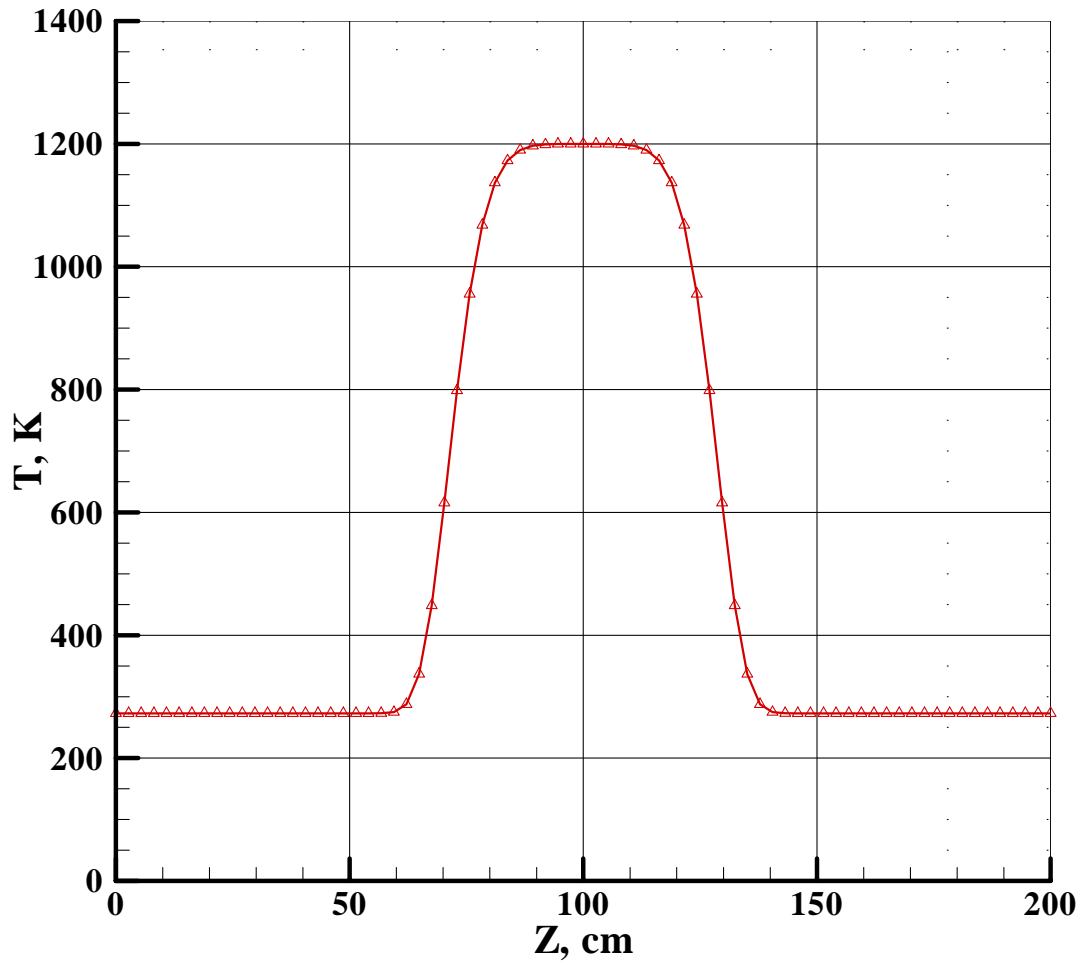


Fig.17. Problem II: Axial temperature distribution in 3D Cartesian coordinates

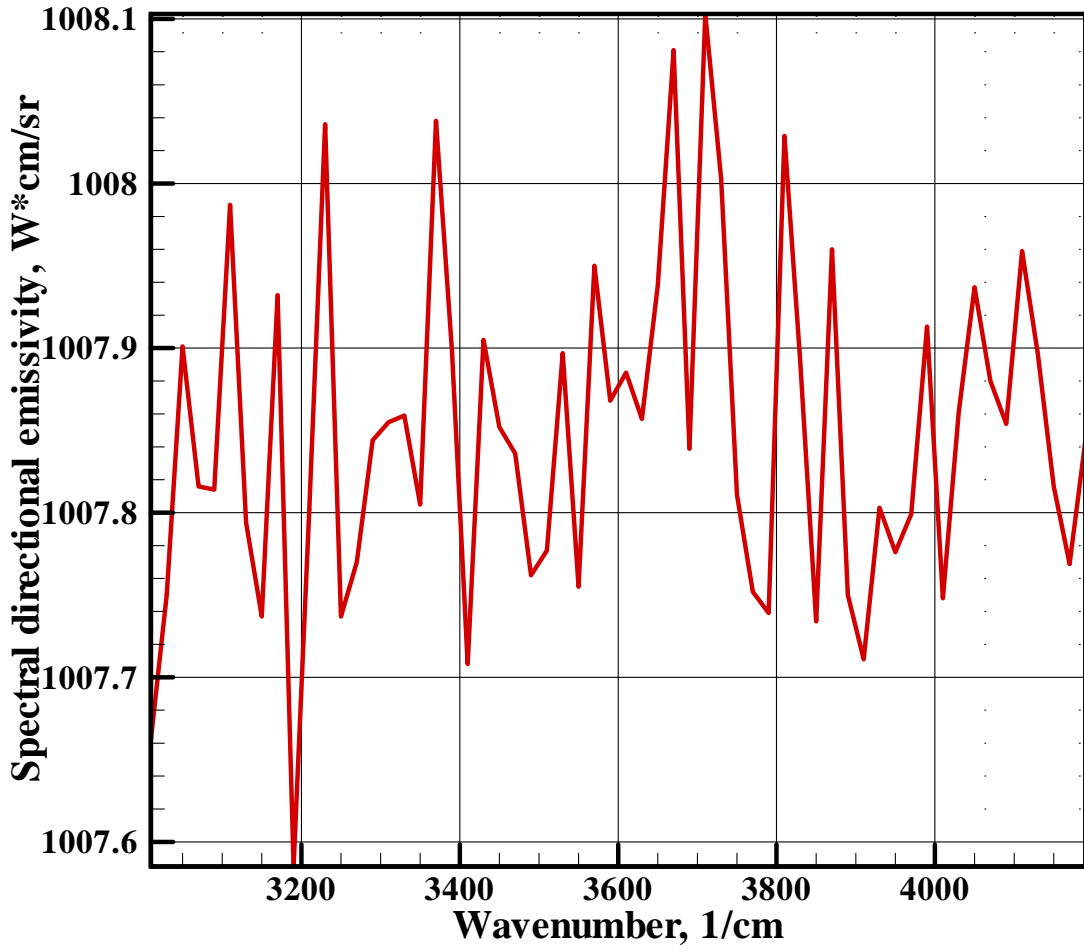


Fig. 18. Problem II: Spectral signature of homogeneous spherical volume in 3D geometry, $N_{ph}=10^5$, $\theta=0$

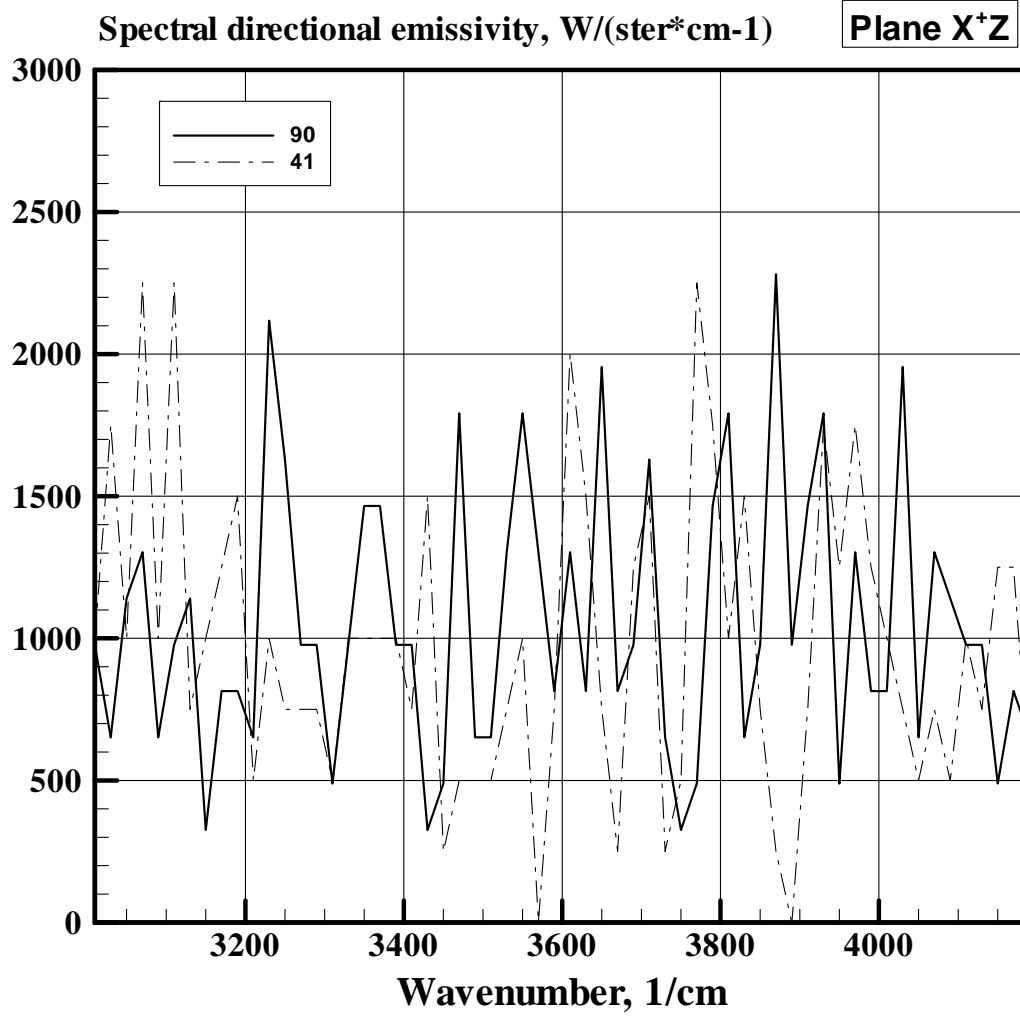


Fig. 19. Problem II: Spectral signature of homogeneous spherical volume in 3D geometry, the integral estimation algorithm (MCIEDE), $N_{ph}=10^5$, $\theta=0$

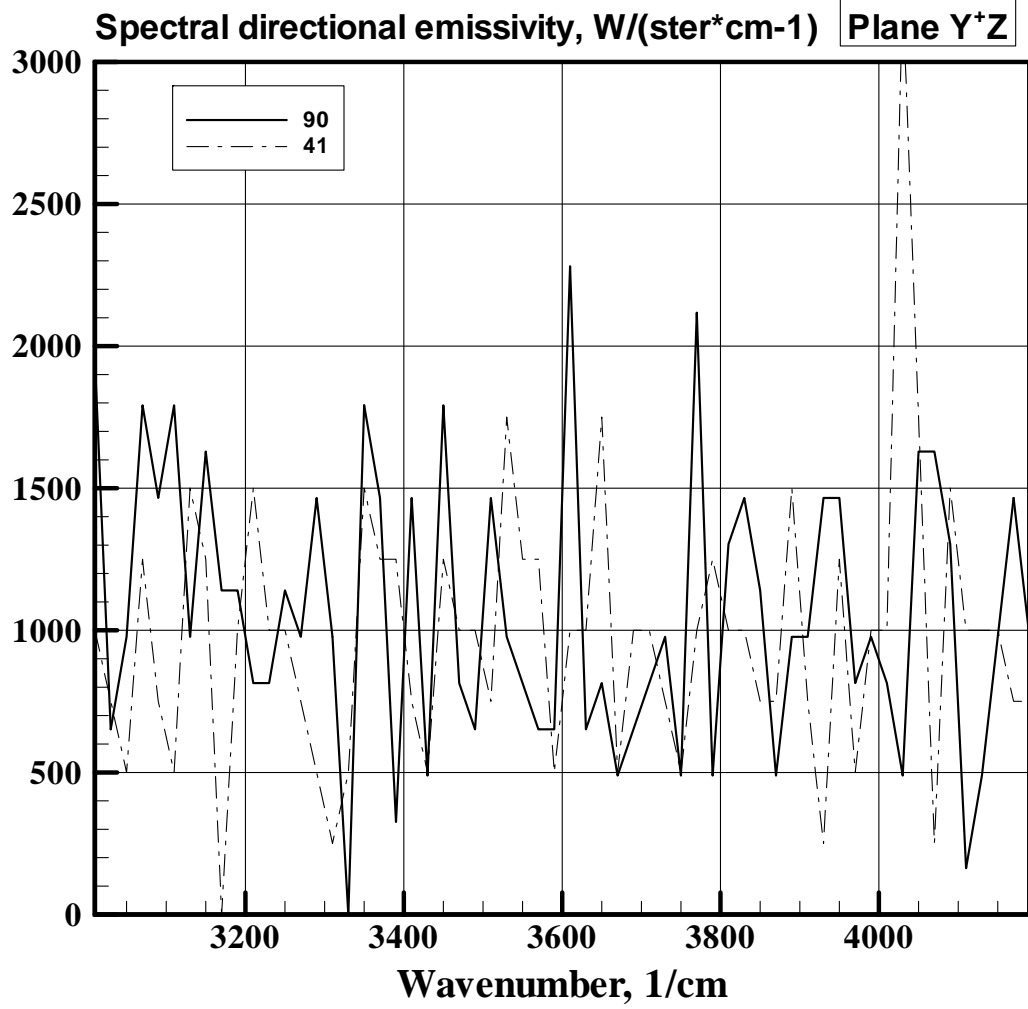


Fig. 20. Problem II: Spectral signature of homogeneous spherical volume in 3D geometry, the integral estimation algorithm (MCIEDE), $N_{ph}=10^5$, $\theta=90$

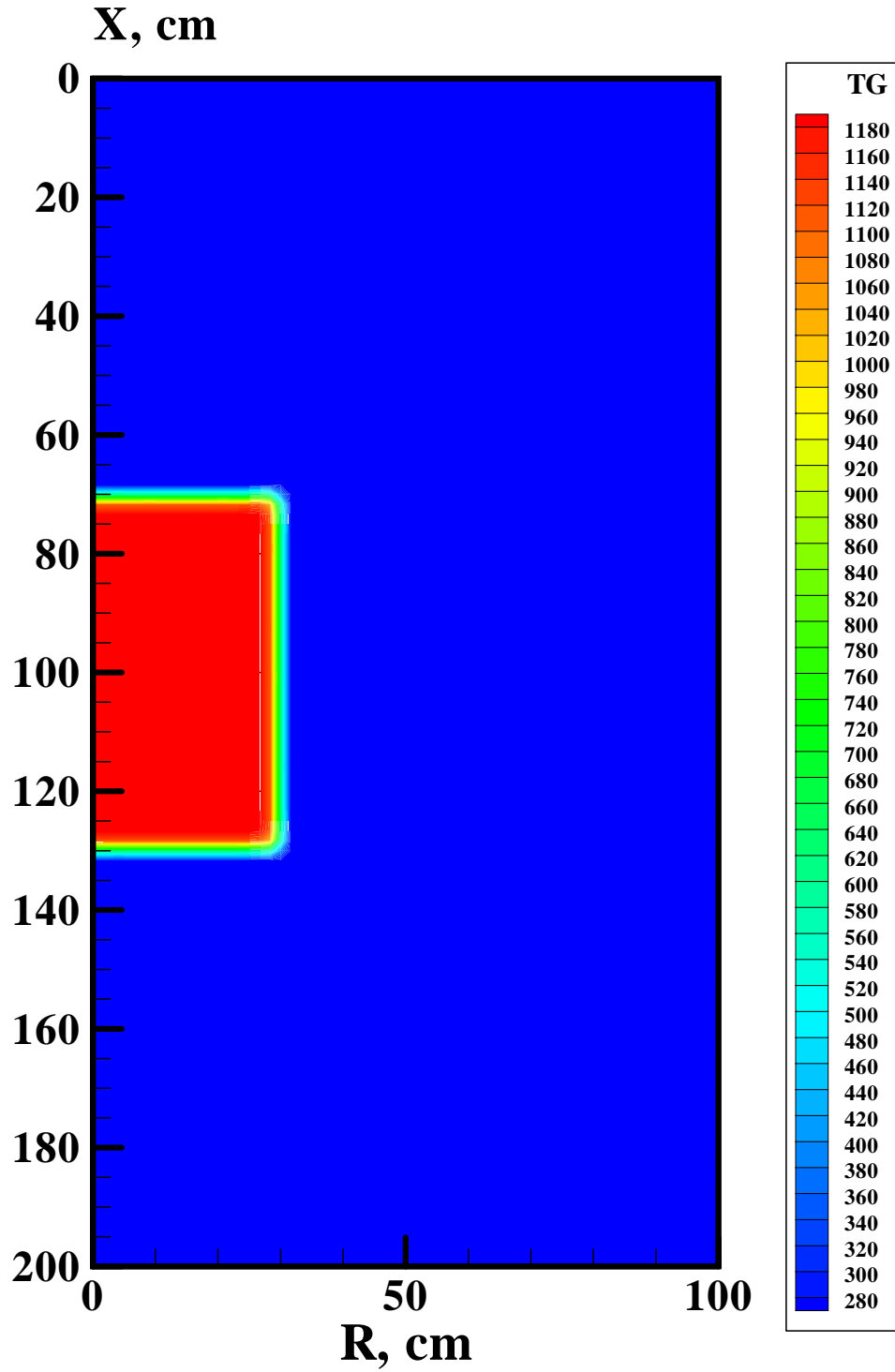


Fig.21. Problem III: Temperature field of cylindrical form in axisymmetric cylindrical geometry

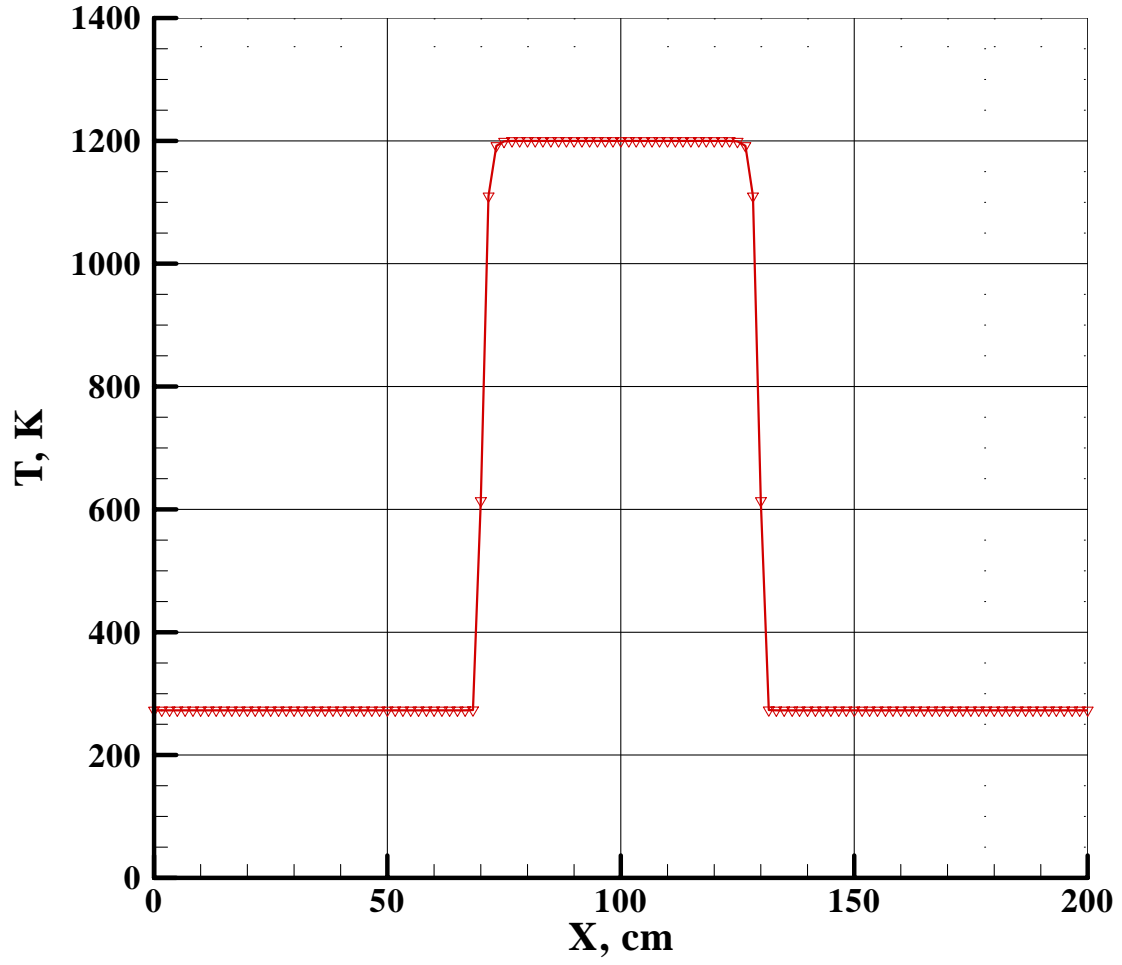


Fig.22. Problem III: Temperature distribution along axis of symmetry of cylindrical volume

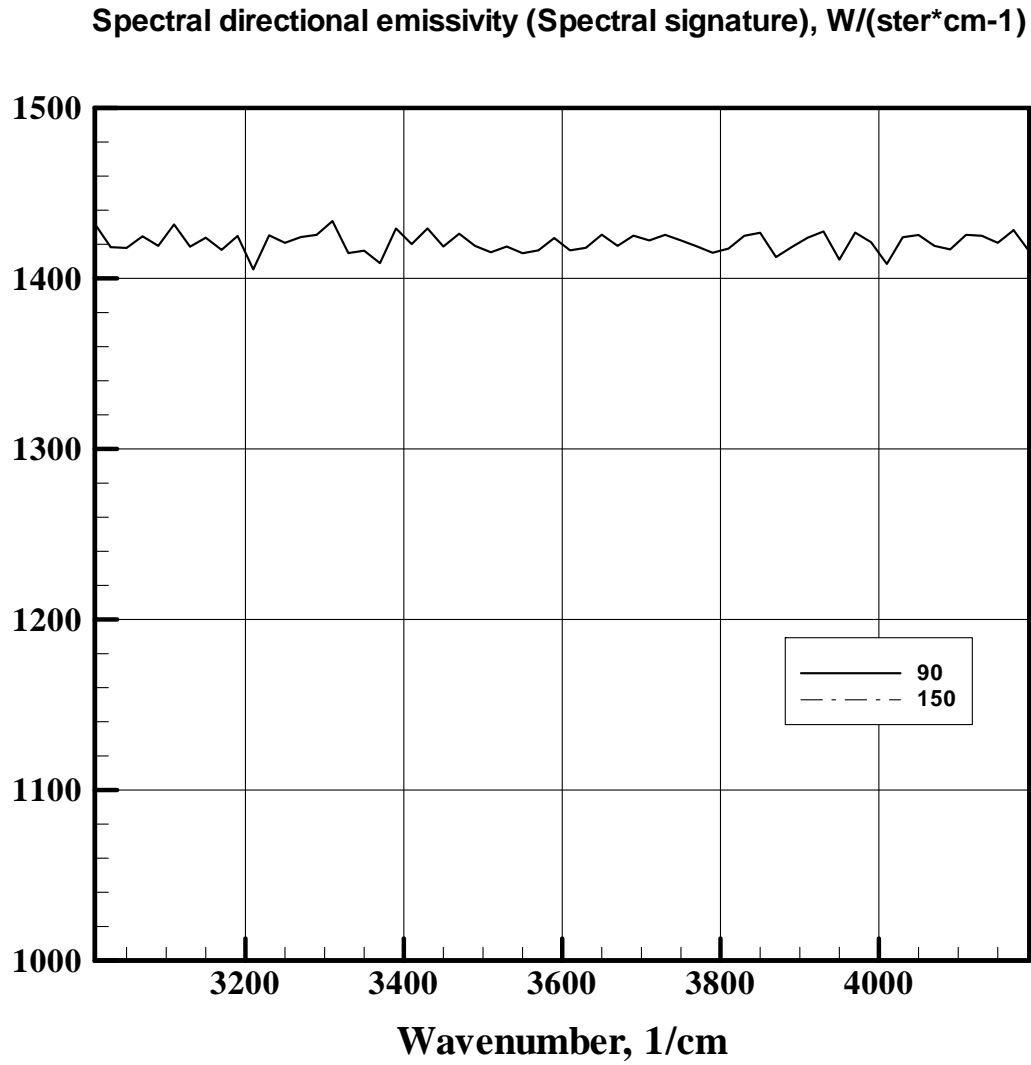


Fig. 23. Problem III: Spectral signature of homogeneous cylindrical volume from the cylindrical surface, $N_{ph}=10^6$; Code Plume-2D-MC

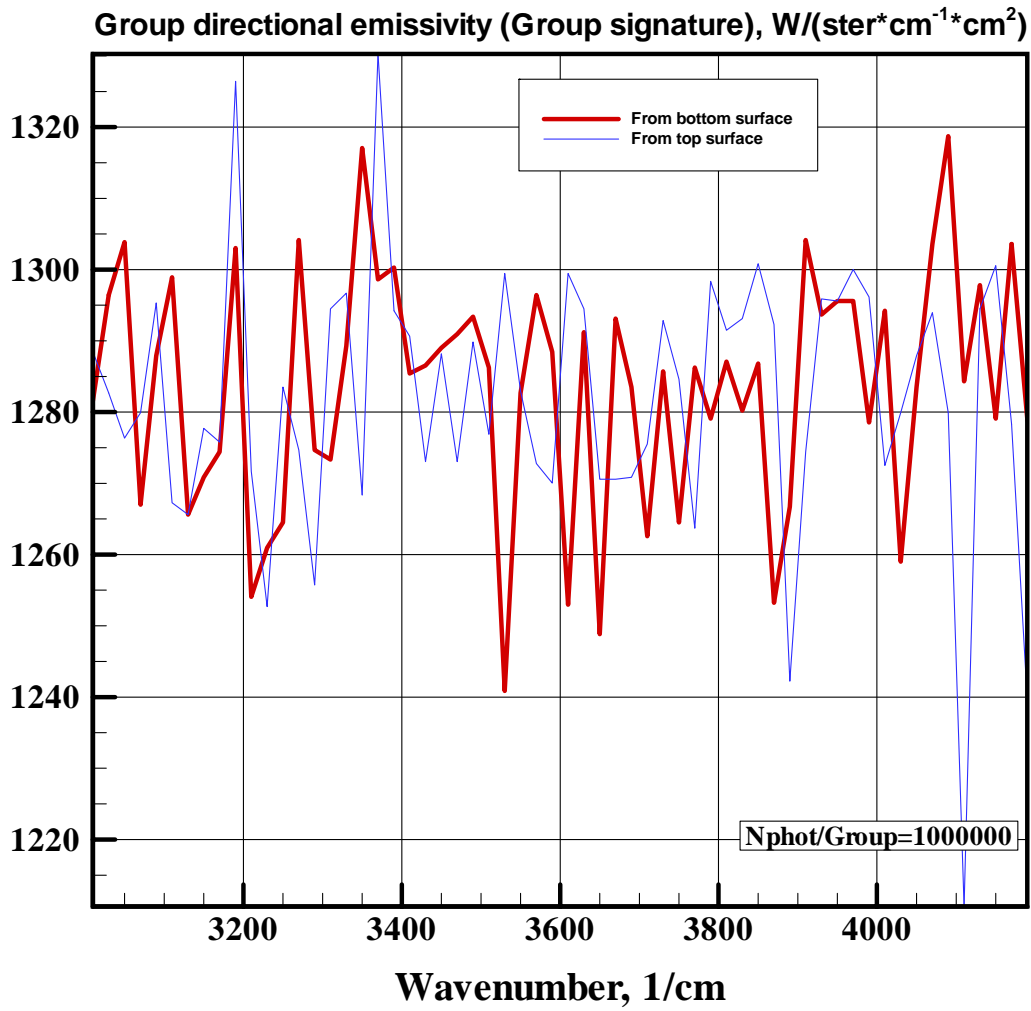


Fig. 24. Problem III: Spectral signature of homogeneous cylindrical volume from plane surfaces, $N_{ph} = 10^5$; Code Plume-2D-MC

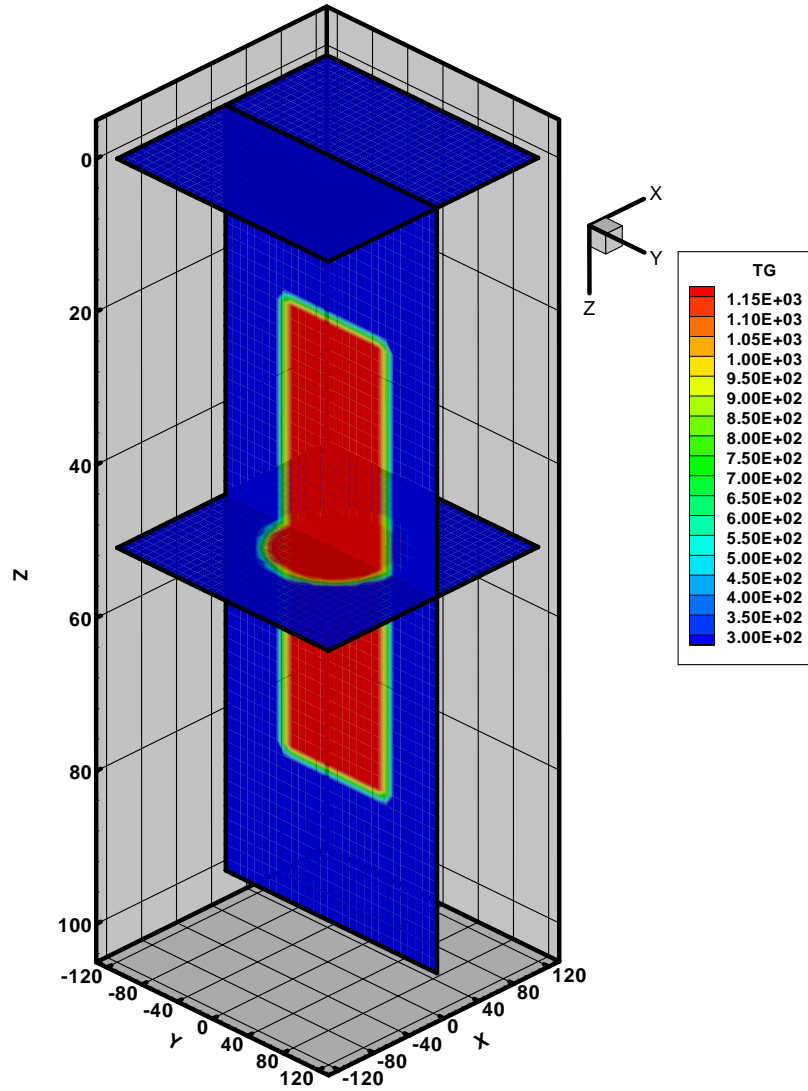


Fig.25. Problem III: Temperature field of heated cylinder in 3D Cartesian coordinates

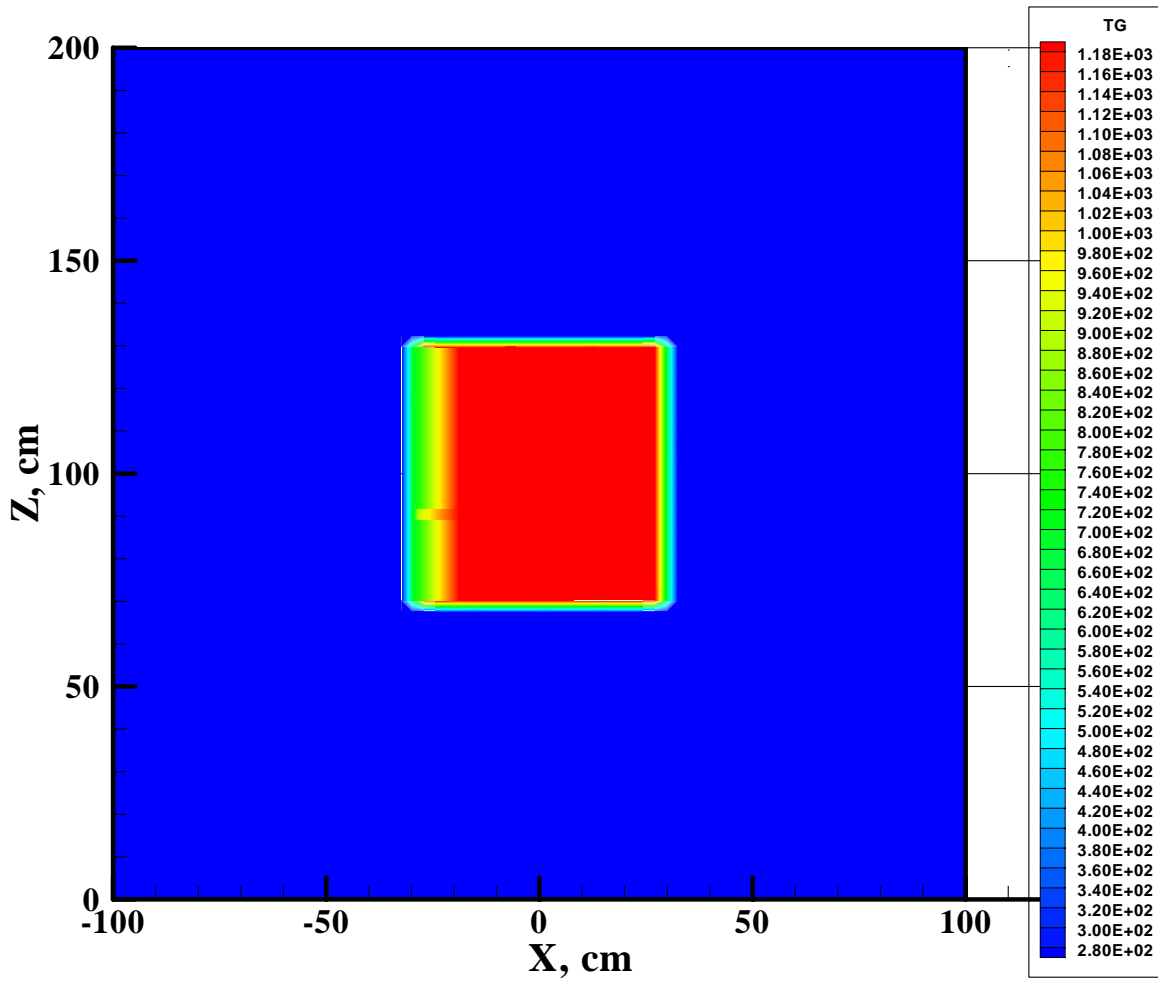


Fig. 26. Problem III: Side view of temperature field of heated cylinder in 3D Cartesian coordinates

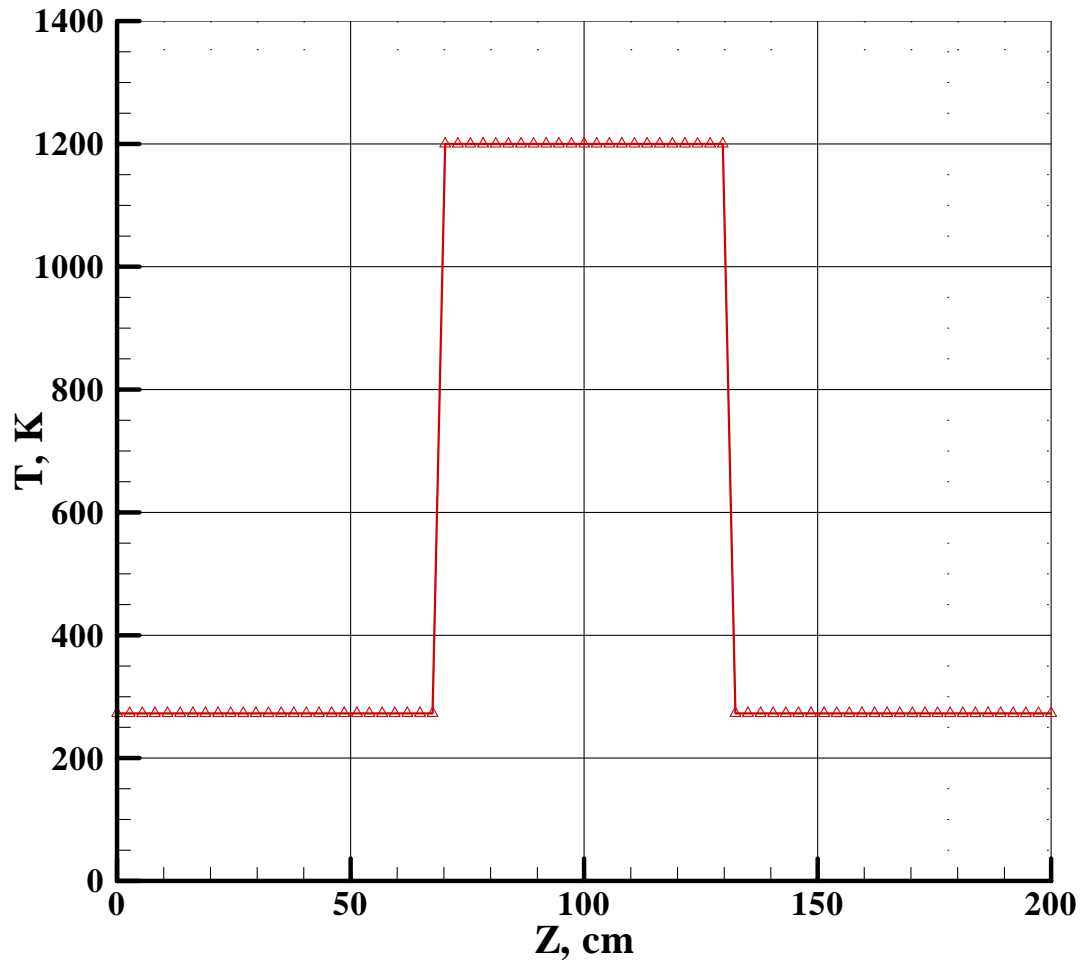


Fig.27. Problem III: Temperature distribution along axis of symmetry of heated cylinder in 3D geometry

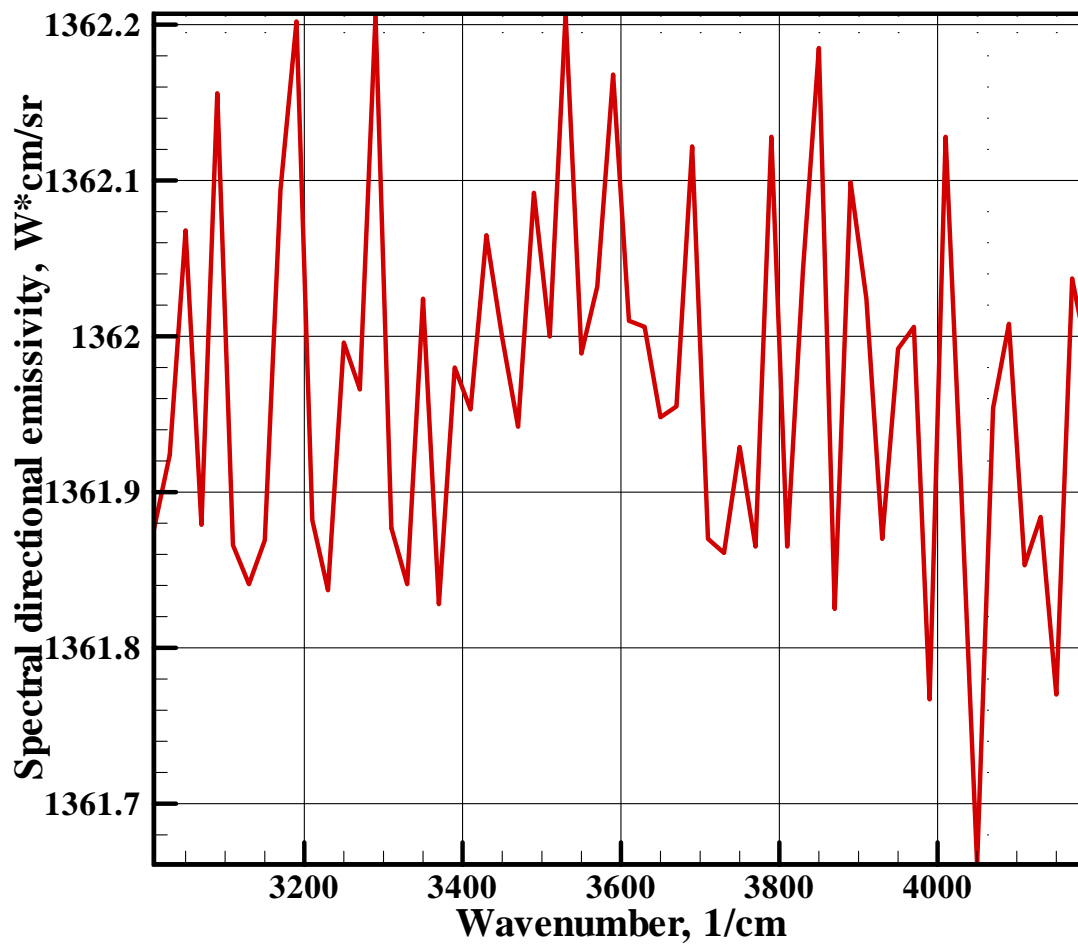


Fig. 28. Problem III: Spectral signature of homogeneous cylindrical volume from the side of cylindrical surface in 3D Cartesian coordinates, $N_{ph} = 10^4$; MCLEDE algorithm;
Code Plume-3D-MC

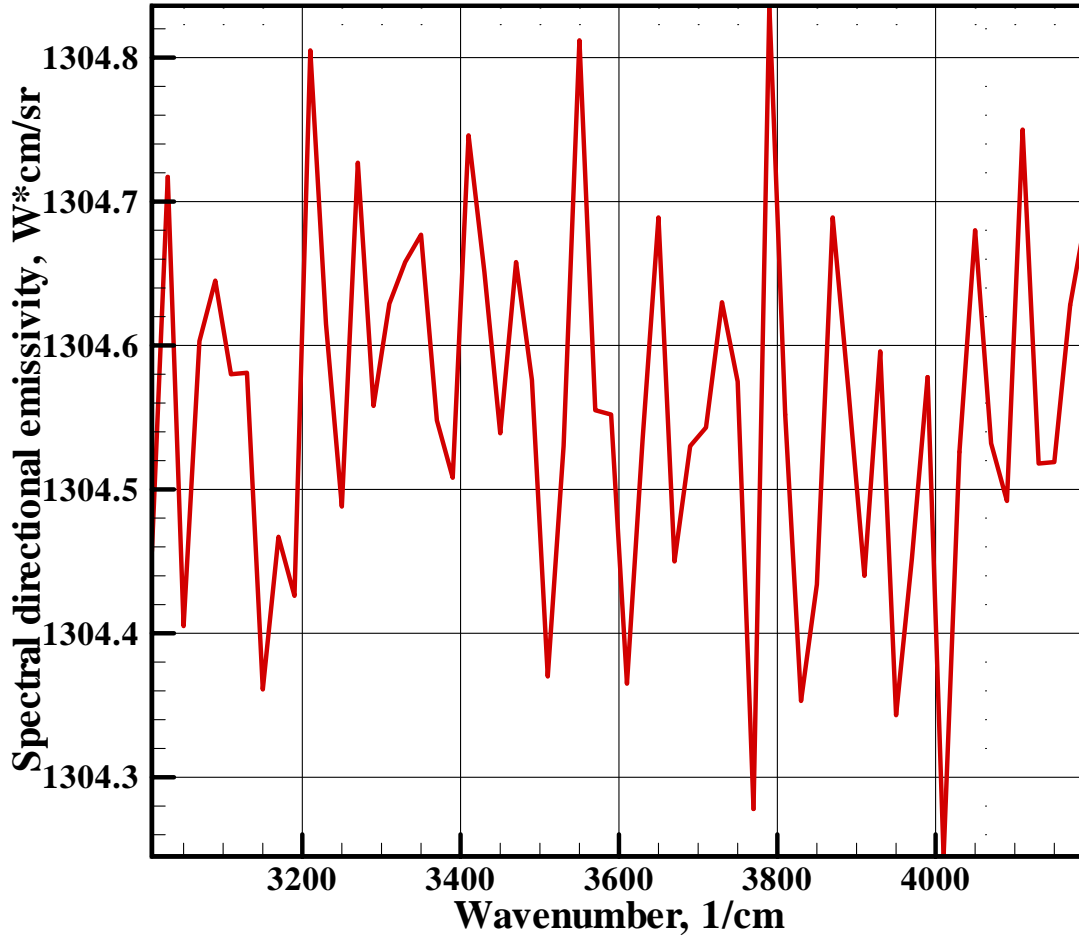


Fig. 29. Problem III: Spectral signature of homogeneous cylindrical volume from the side of plane surfaces in 3D Cartesian coordinates, $N_{ph} = 10^4$; MCLEDE algorithm; Code Plume-3D-MC

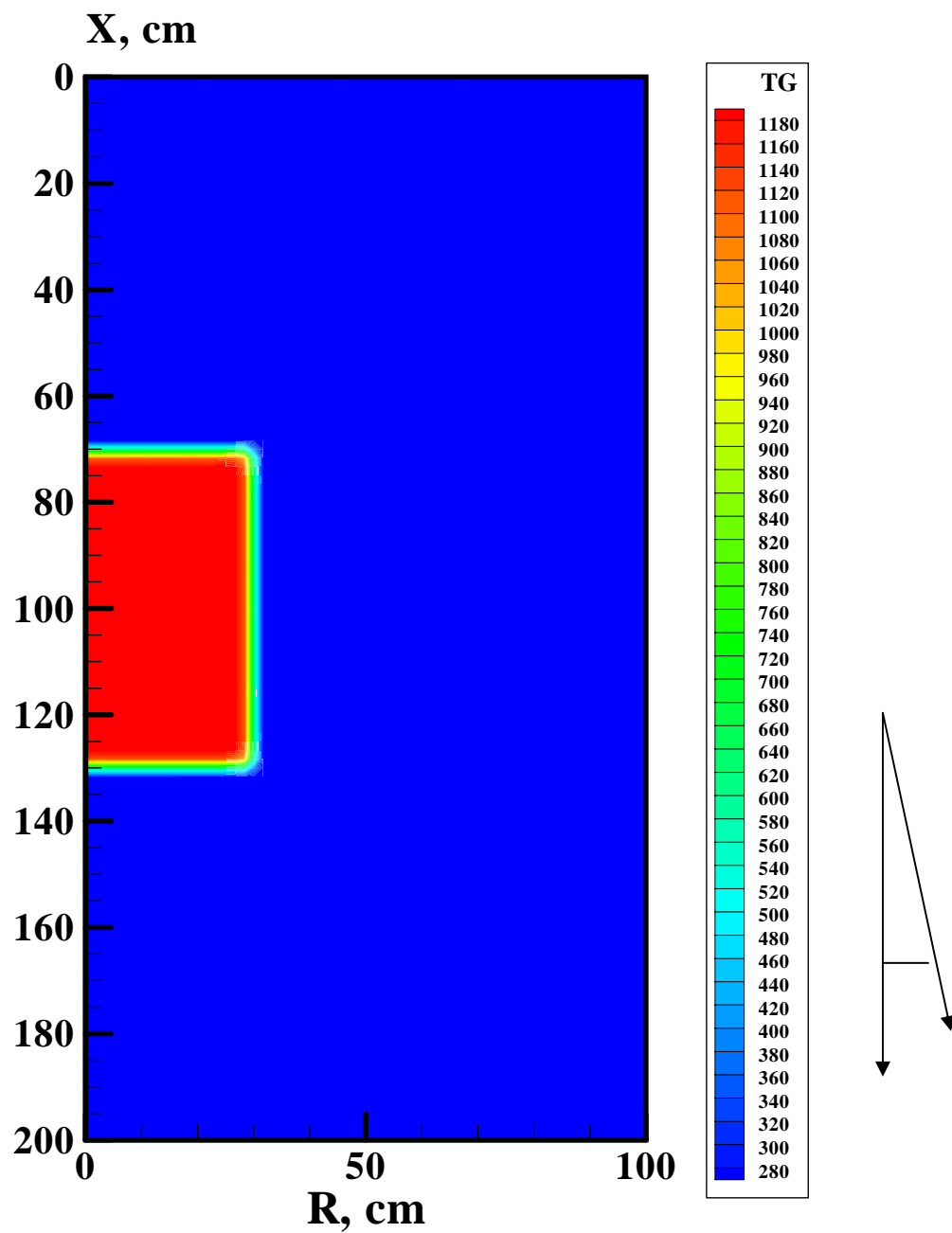


Fig.30. Problem IV: Homogeneous cylindrical volume filled with heated gas mixture at temperature $T=1200$ K. 2D cylindrical geometry.
Direction of observation is $\theta=0$ (the direction is shown in the figure)

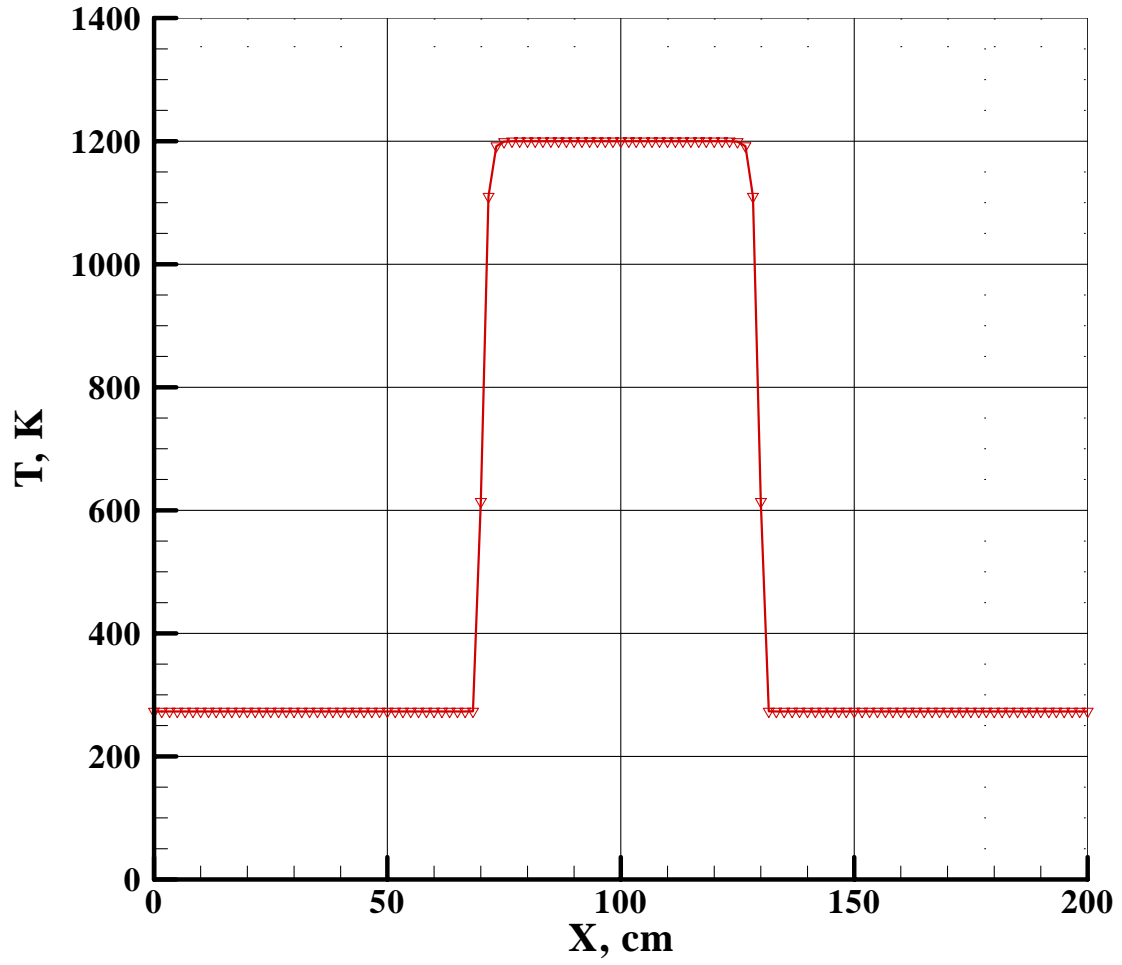


Fig.31. Problem IV: Axial temperature distribution in cylindrical calculation domain

θ

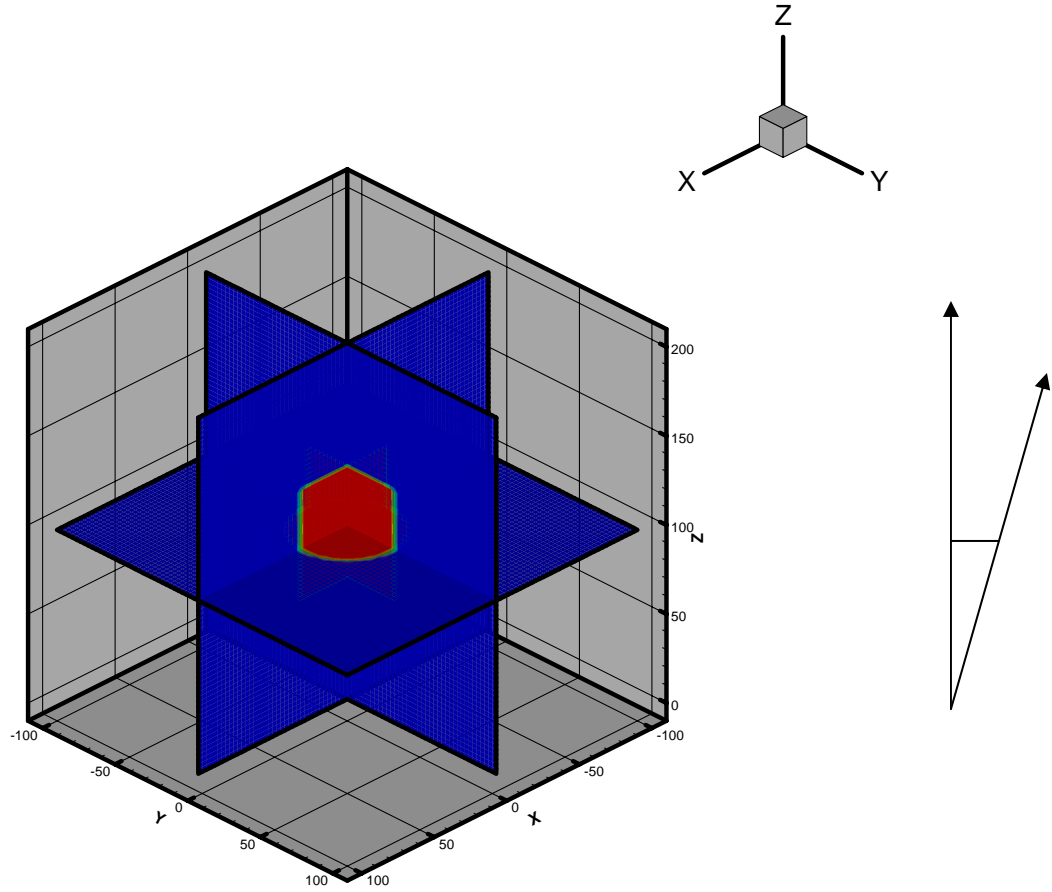


Fig.32. Problem IV: Homogeneous cylindrical volume filled with heated gas mixture at temperature $T = 1200$ K. 3D Cartesian coordinate system. Direction of observation is $\theta=0$ (the direction is shown in the figure)

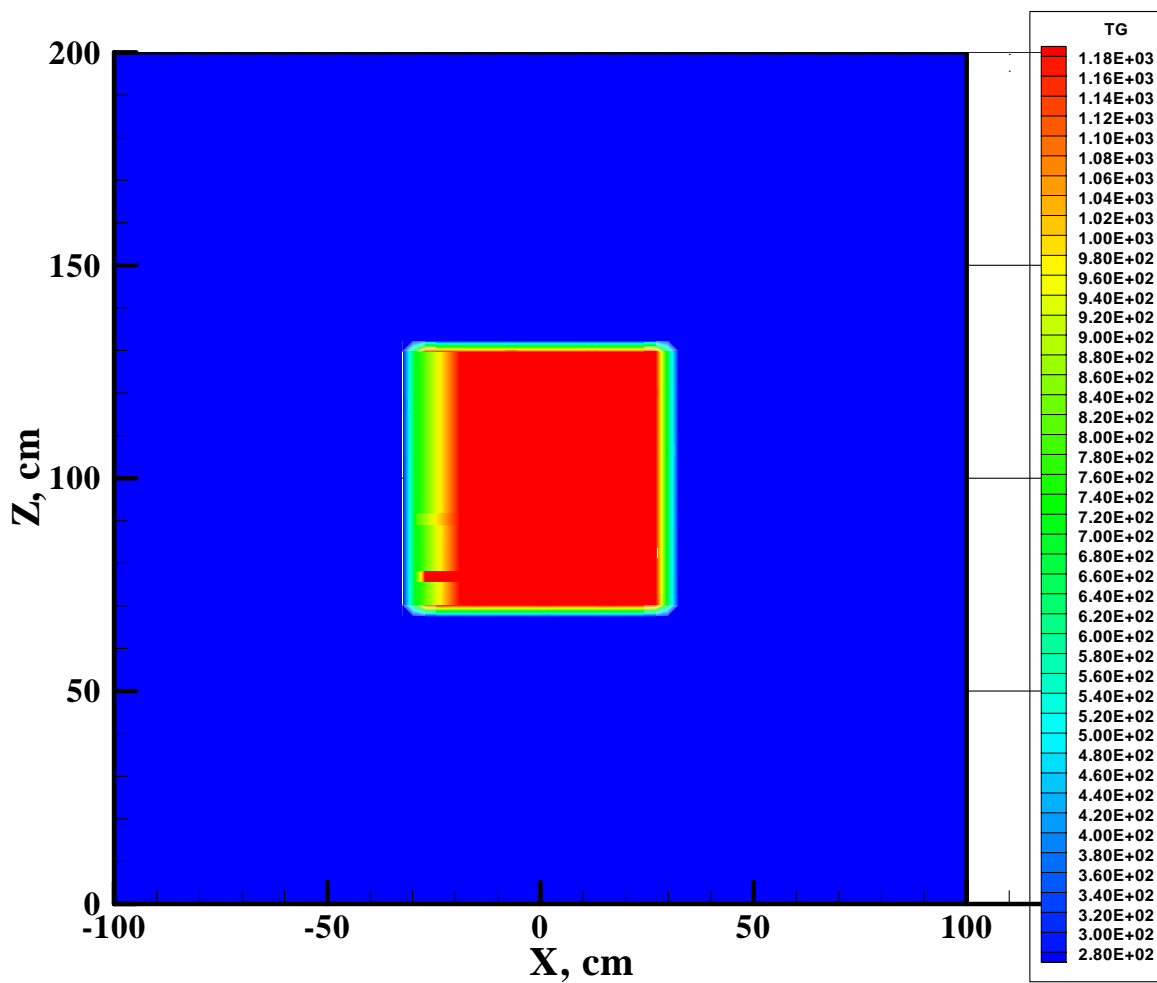


Fig.33. Problem IV: Side view of homogeneous cylindrical volume filled with heated gas mixture at temperature $T=1200$ K. 3D Cartesian coordinate system.
Direction of observation is $\theta=0$

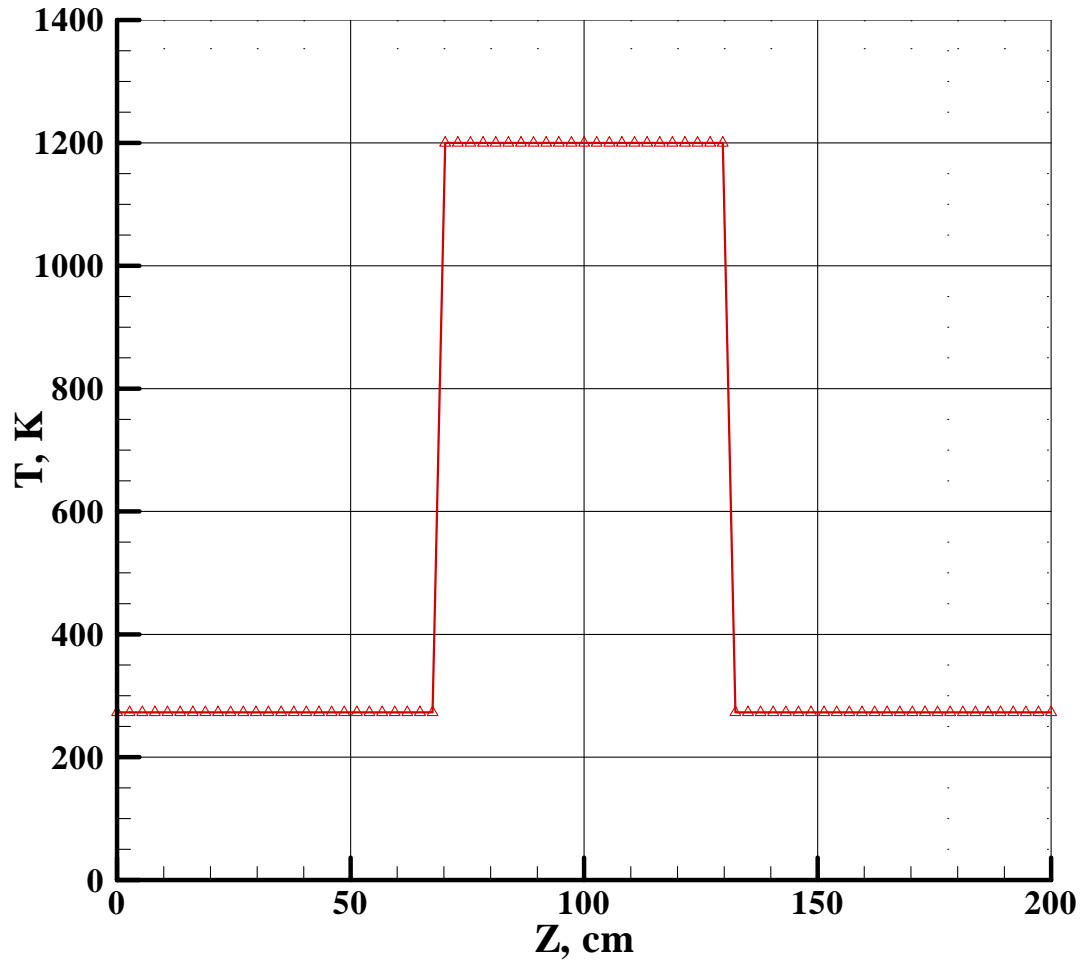


Fig.34. Problem IV: Axial temperature distribution along cylindrical volume of heated gas in 3D Cartesian coordinate system

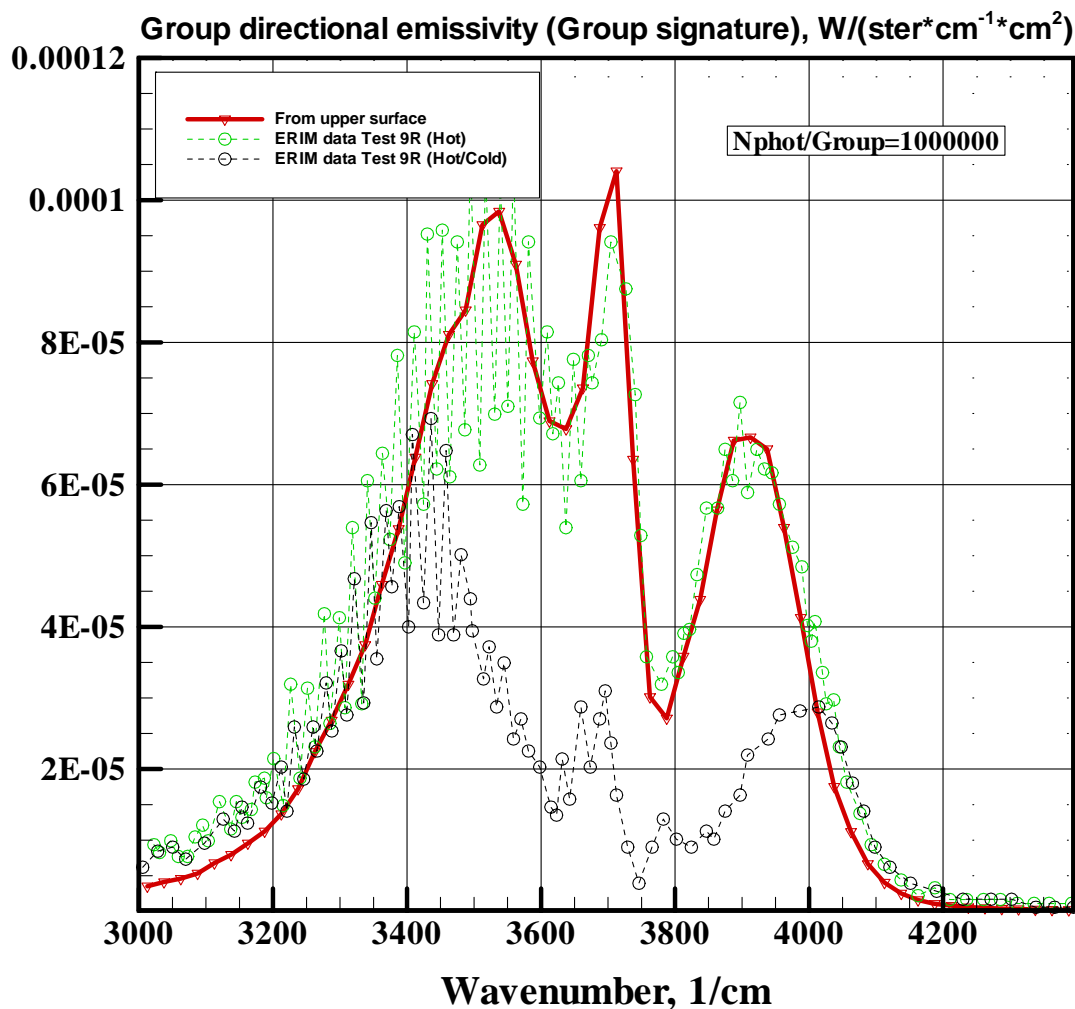


Fig. 35. Problem IV. Test 9R. ERIM experimental data for H₂O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

NASA Standard Infrared Radiation model; averaged rotational line structure (JLBL=0); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$.

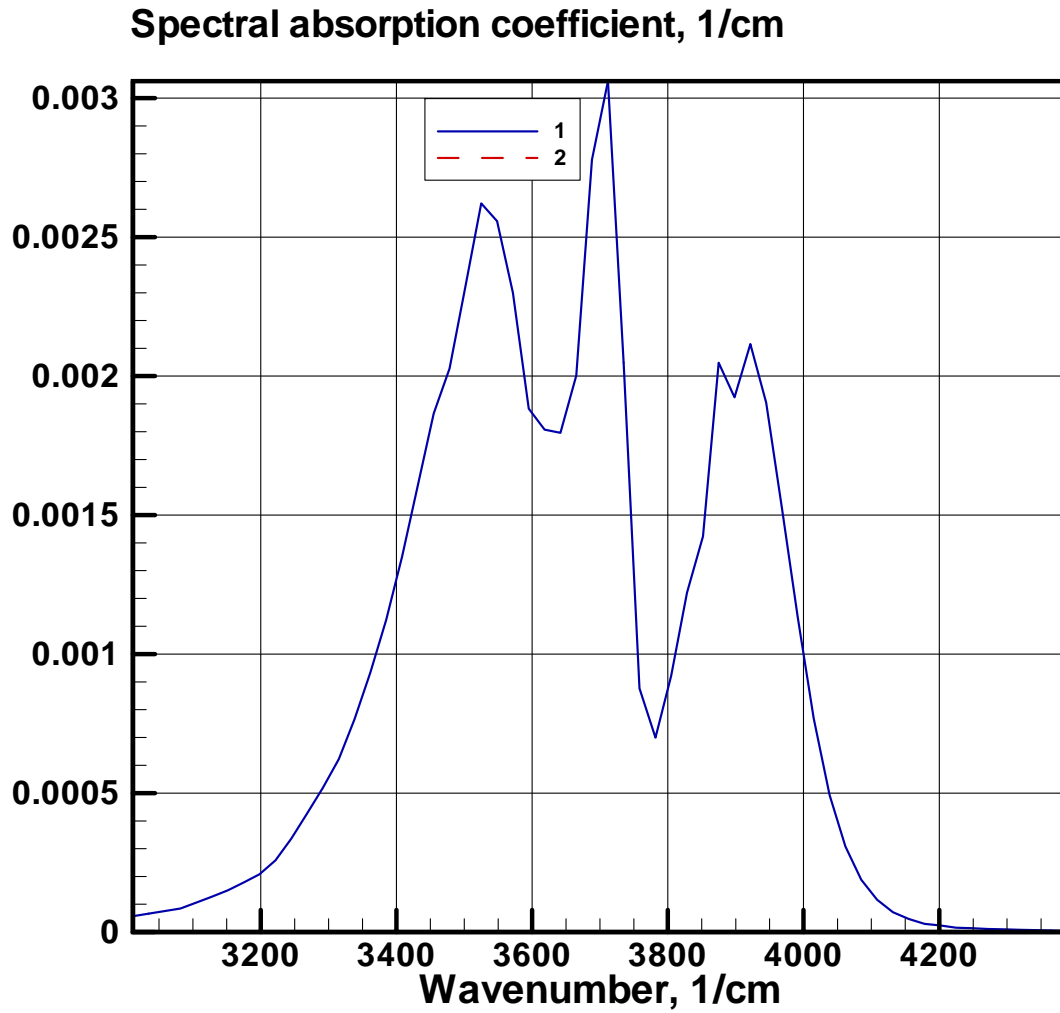


Fig. 36. Problem IV: Spectral absorption coefficient of heated H₂O for conditions of Test 9R.
 Curve No.2 (red dotted line) corresponds to absorption in environment atmosphere ($\kappa_{\omega}=0$).
 The NASA standard infrared radiation model

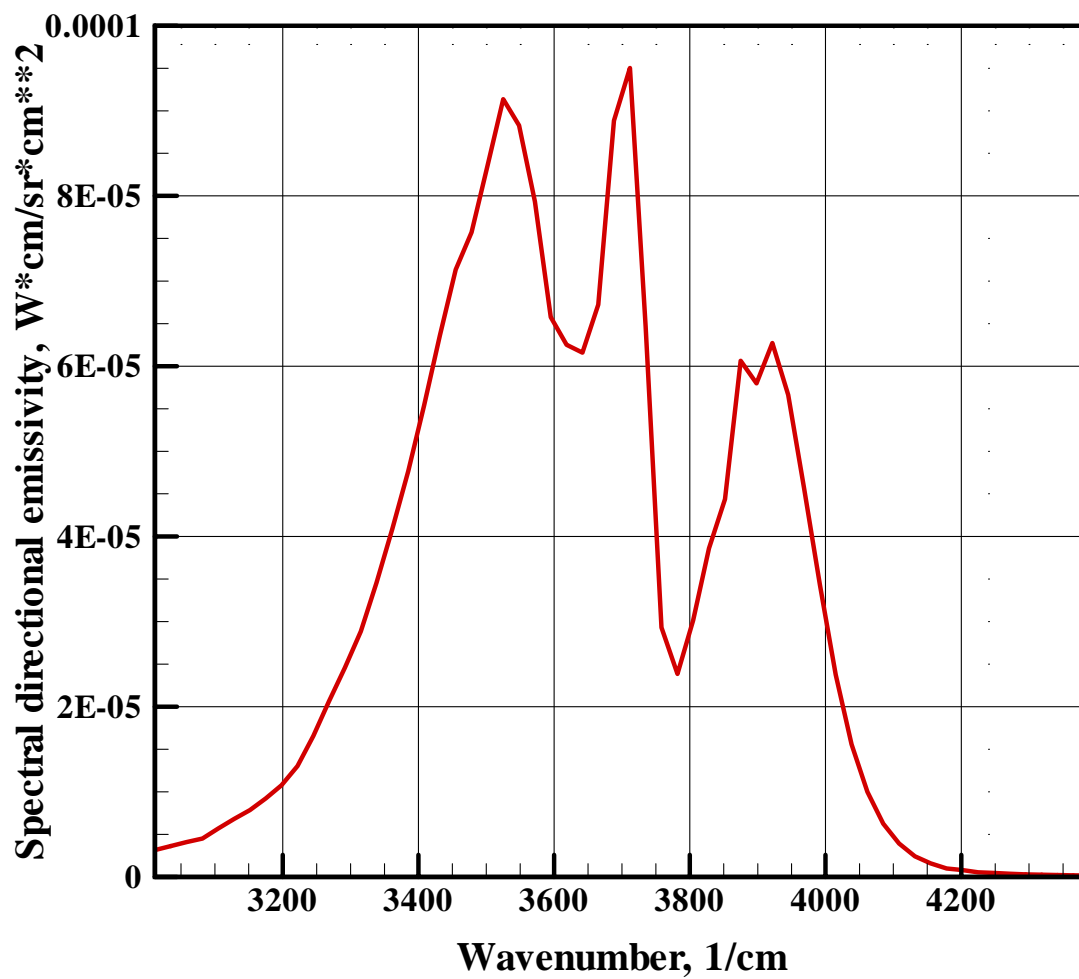


Fig. 37. Problem IV: Spectral signature of homogeneous cylindrical volume heated up to $T = 1200$ K; 3D calculation domain; $N_{ph} = 10^4$; the MCLEDE algorithm.
Code Plume-3D-MC

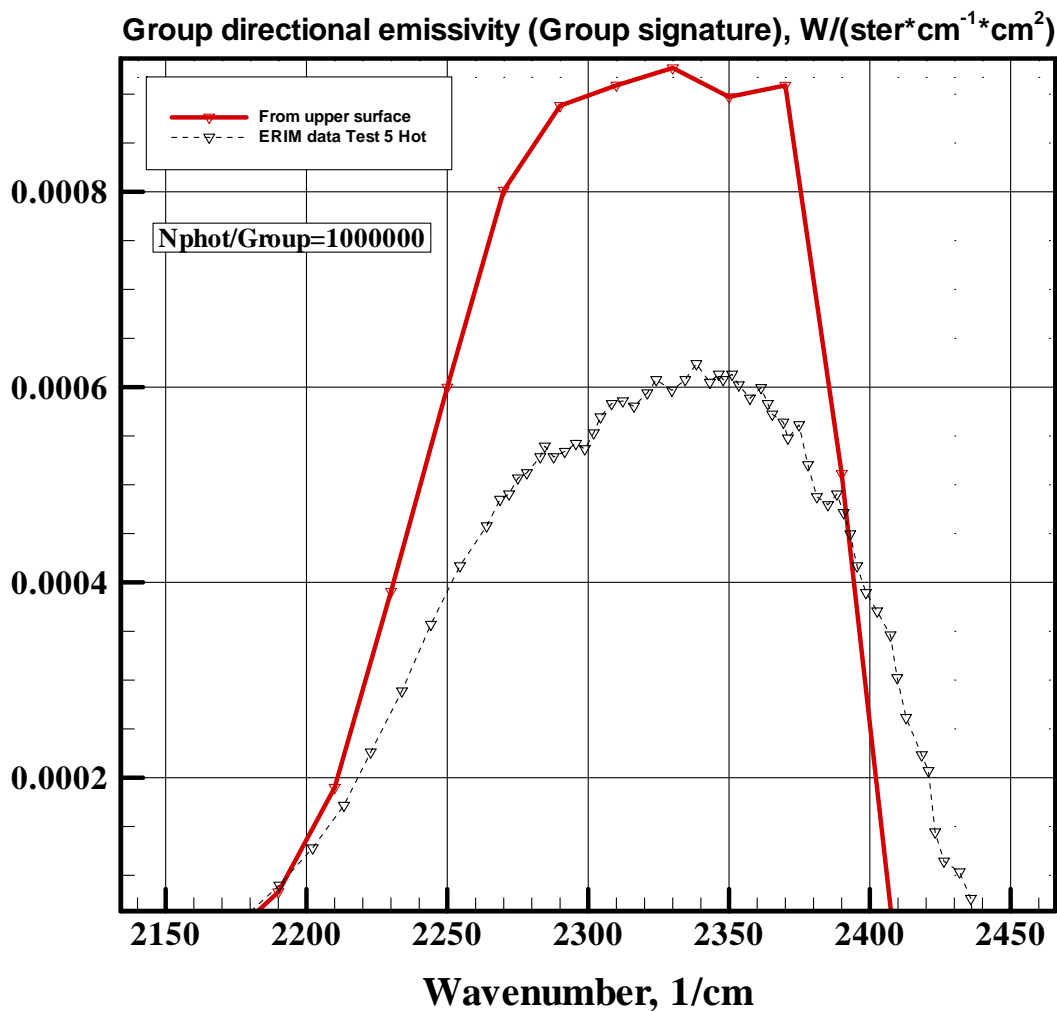


Fig.38. Problem IV. Test 5. ERIM experimental data for CO₂ Hot cell radiance (dotted line) and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The NASA standard infrared radiation model; averaged rotational line structure (JLBL=0; JLBL is the computational flag in code Plume-2D-MC); spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$.

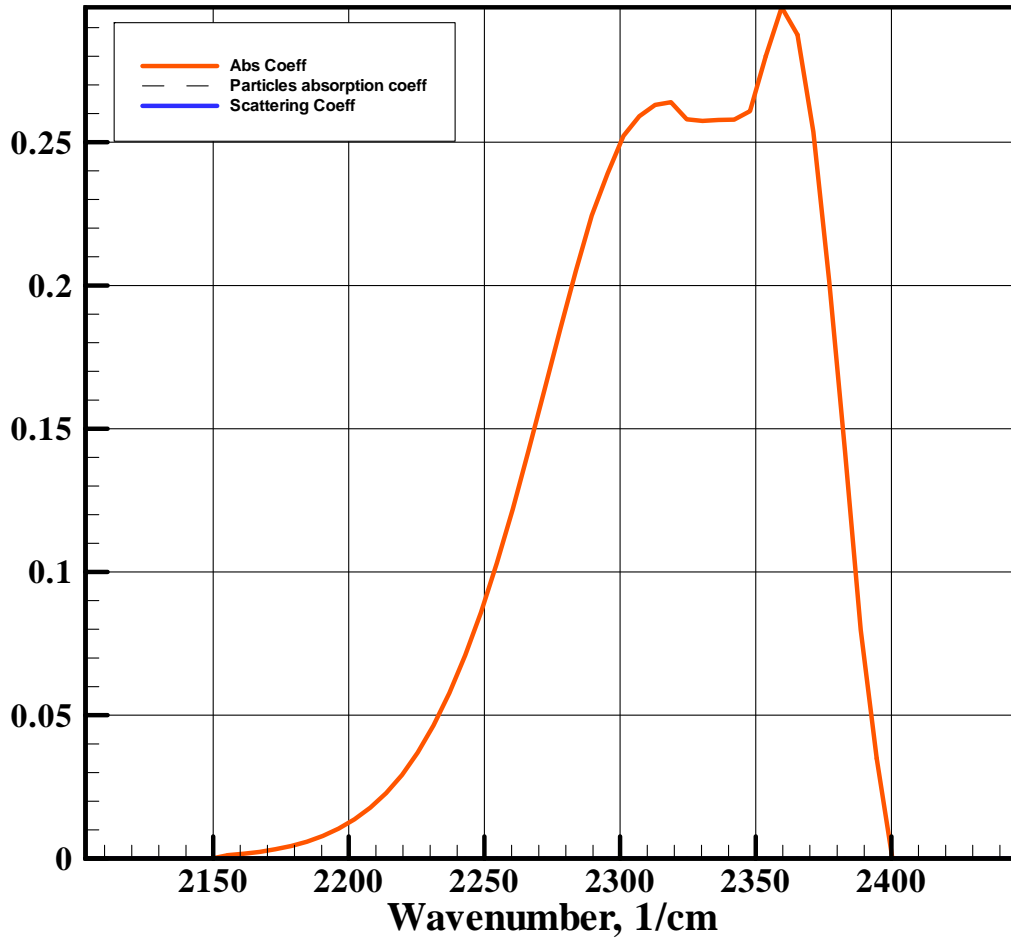


Fig. 39. Problem IV: Spectral absorption coefficient of heated CO₂ at conditions of Test 5; NASA standard infrared radiation model [3]

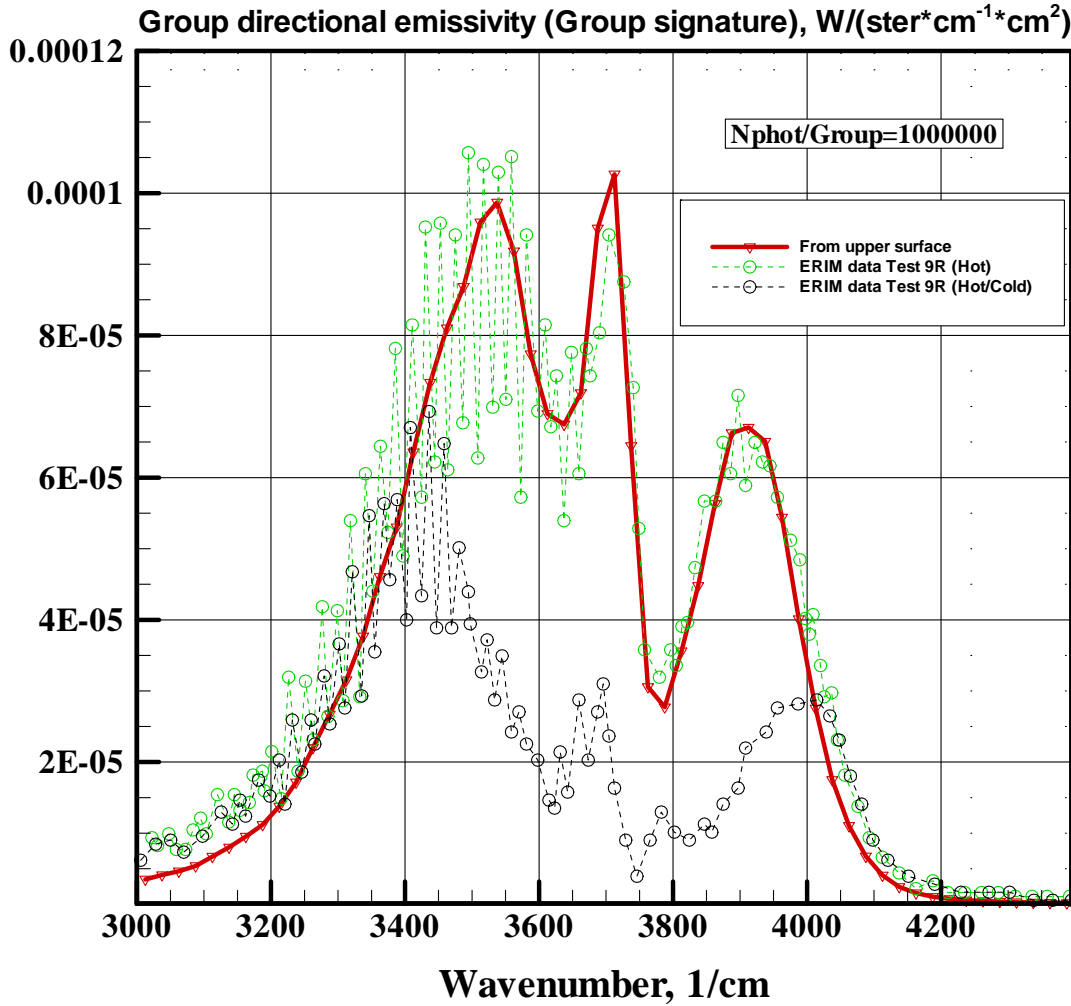


Fig. 40. Problem IV. Test 9R. ERIM experimental data for H_2O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The NASA standard infrared radiation model; narrow-band random model (JLBL=2; JLBL is the computational flag in computing code Plume-2D-MC); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$.

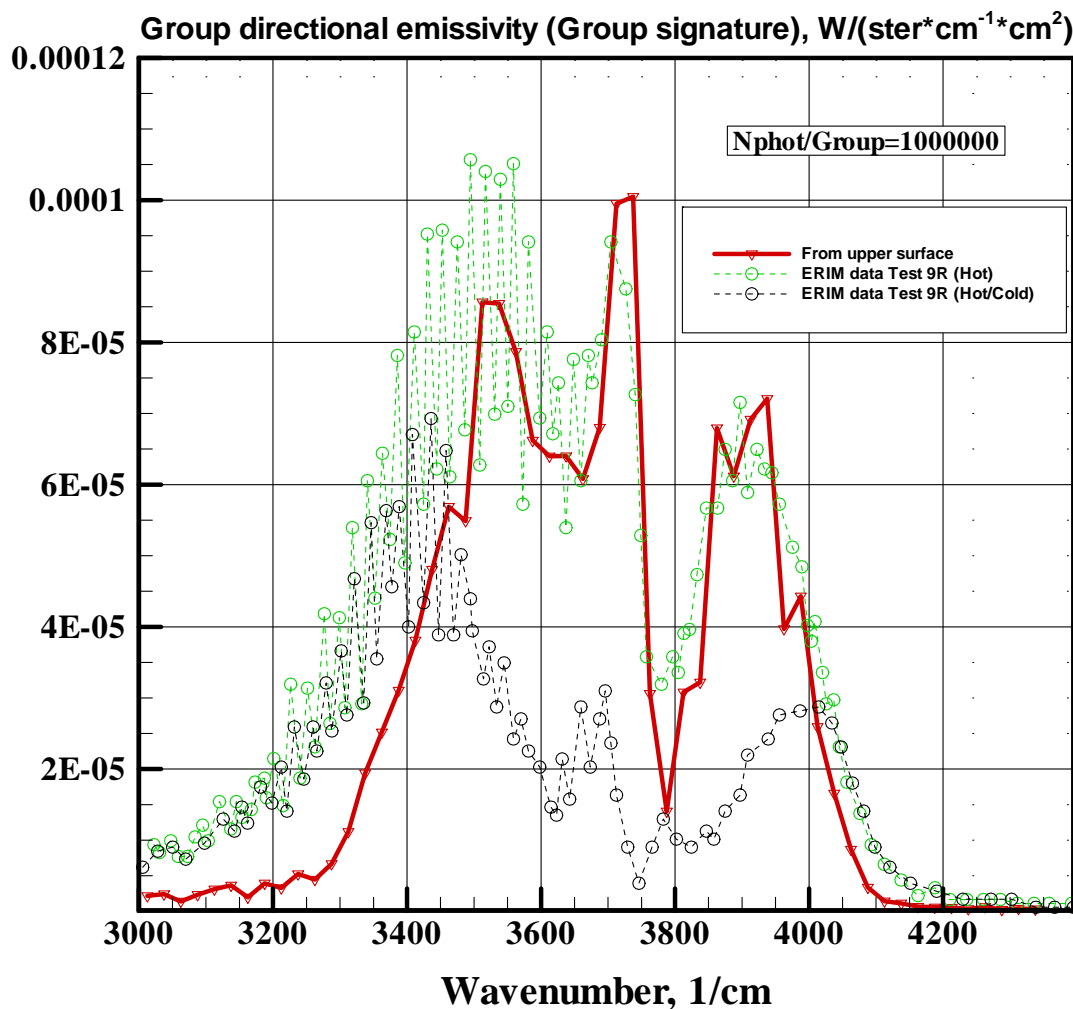


Fig.41. Problem IV. Test 9R. ERIM experimental data for H_2O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The HITRAN temperature-extrapolated data; averaged rotational line structure (JLBL=0, JSUM=1); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

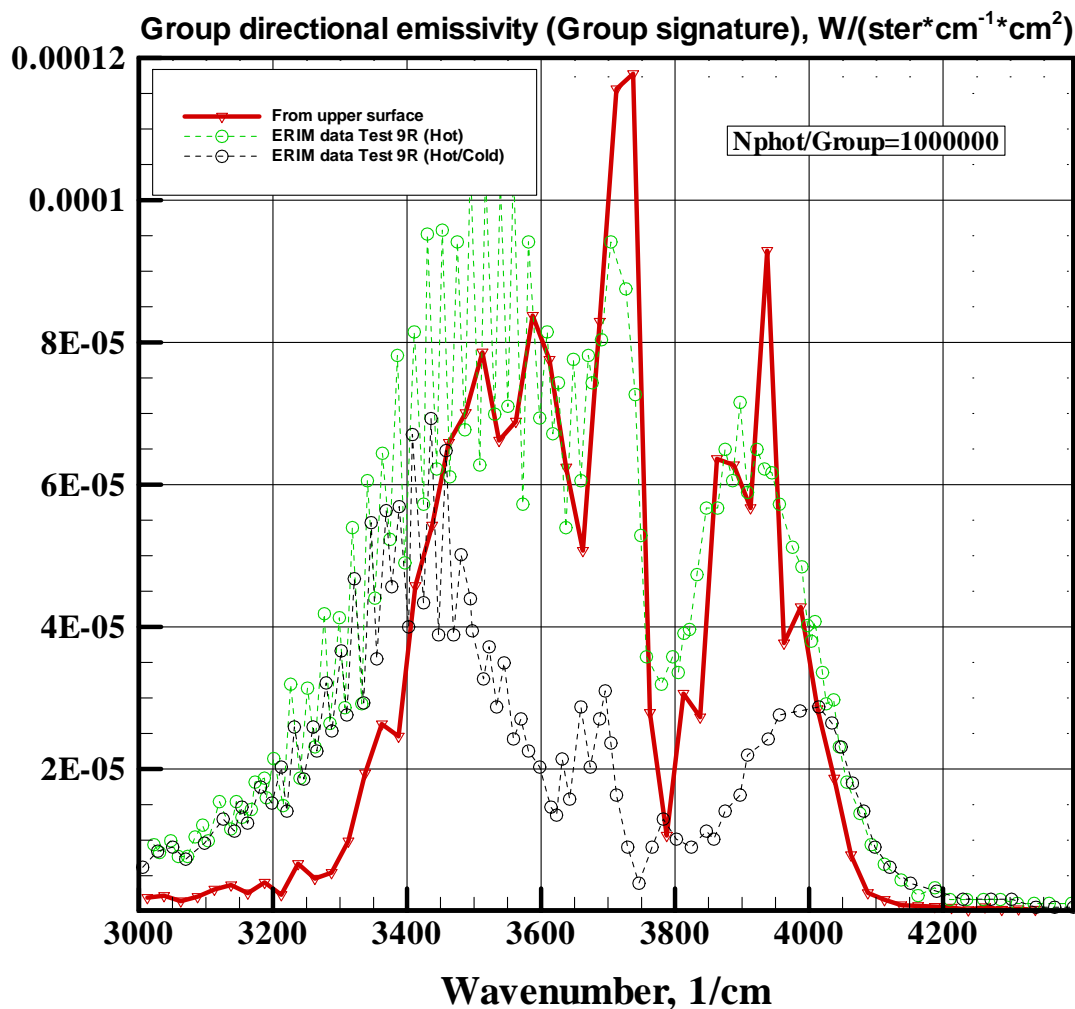


Fig.42. Problem IV. Test 9R. ERIM experimental data for H_2O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The HITRAN temperature-extrapolated data; averaged rotational line structure (JLBL=0, JSUM=0); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

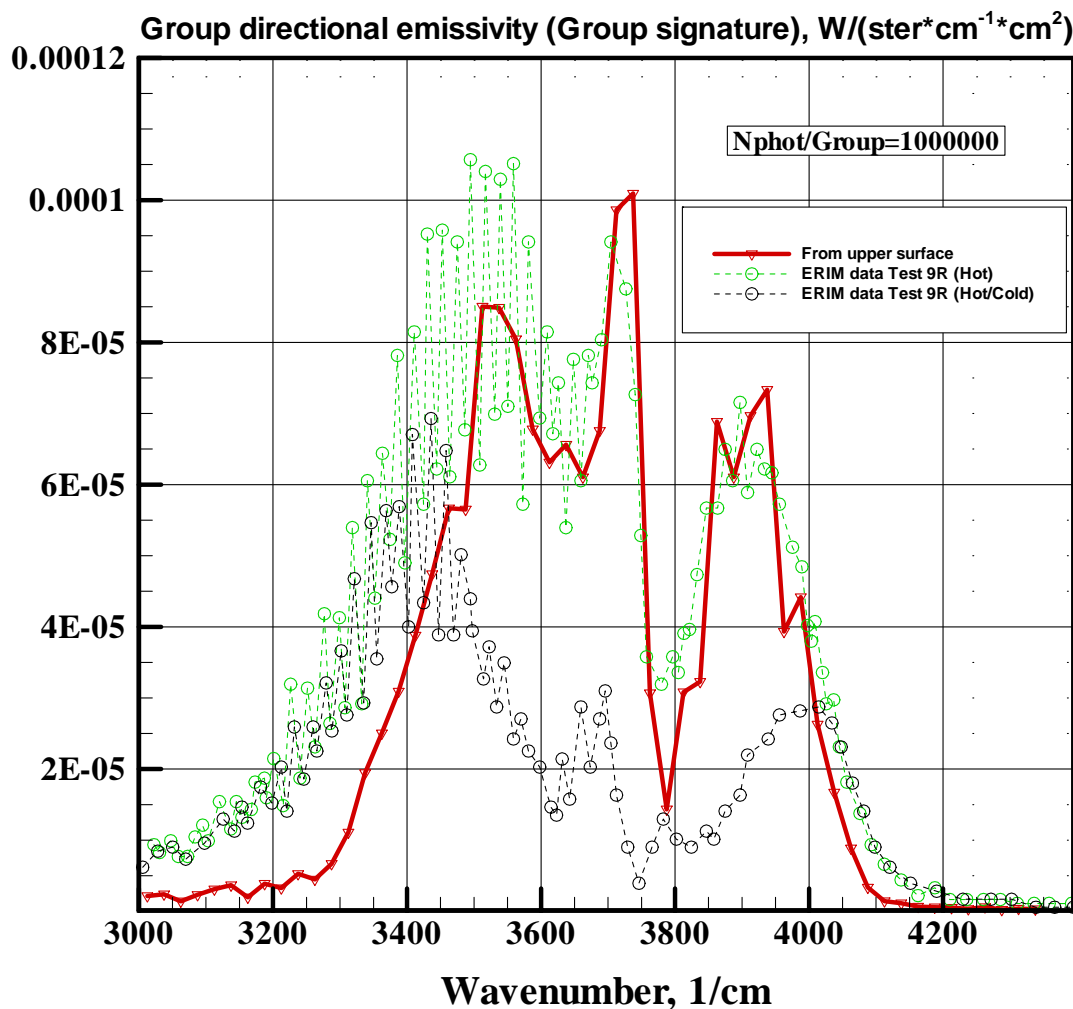


Fig.43. Problem IV. Test 9R. ERIM experimental data for H_2O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The HITRAN temperature-extrapolated data; random model (JLBL=3); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

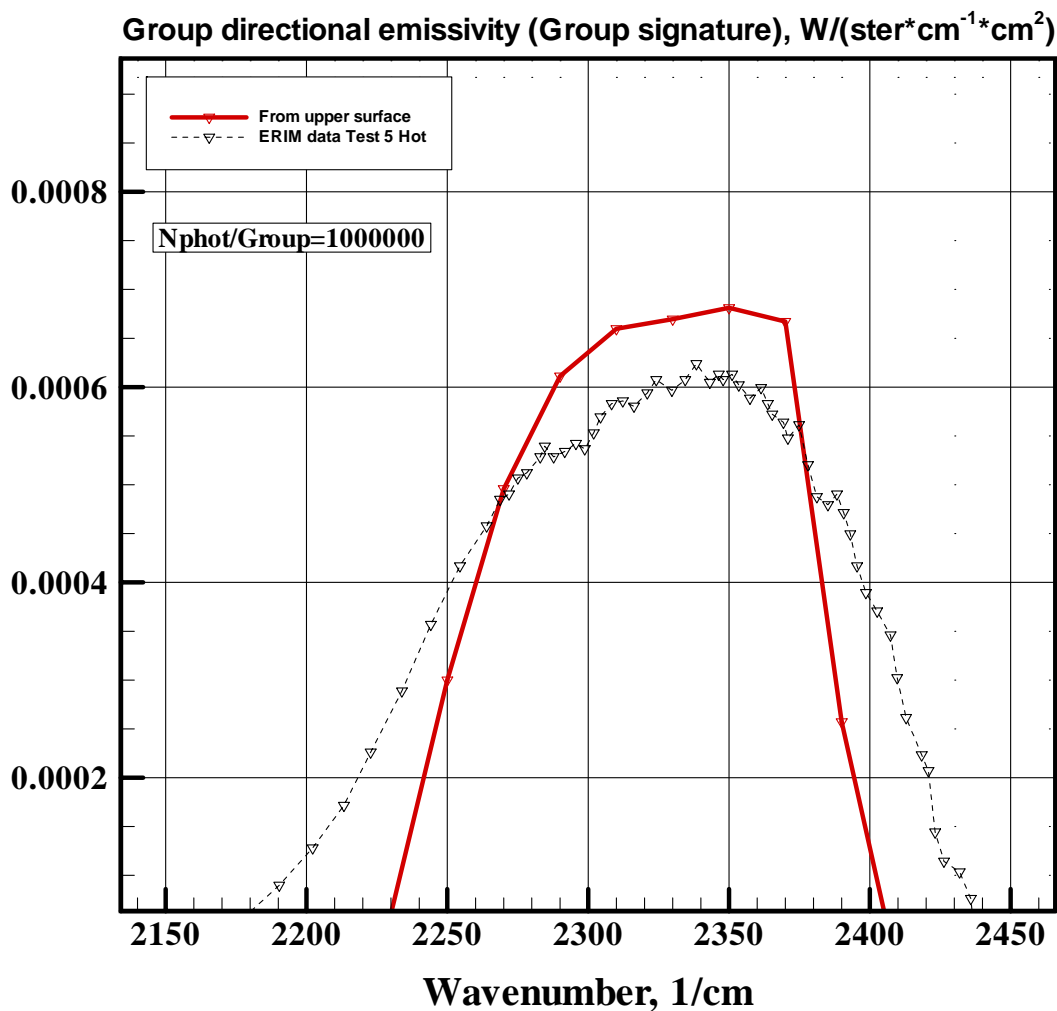


Fig.44. Problem IV. Test 5. ERIM experimental data for CO₂ Hot cell radiance (dotted line) and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

HITRAN temperature-extrapolated data; averaged rotational line structure (JLBL=0, JSUM=1); spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$

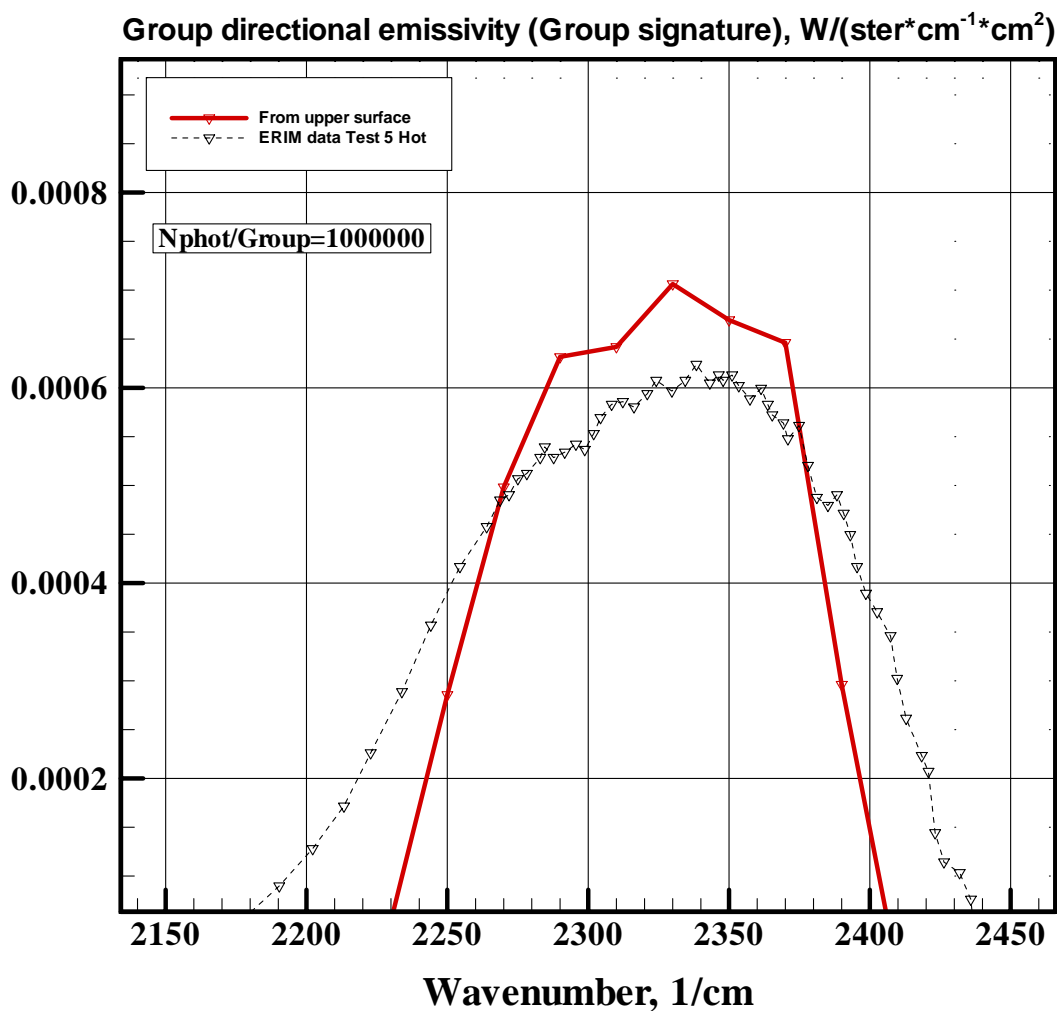


Fig.45. Problem IV. Test 5. ERIM experimental data for CO₂ Hot cell radiance (dotted line) and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

HITRAN temperature-extrapolated data; averaged rotational line structure (JLBL=0, JSUM=2);
spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$

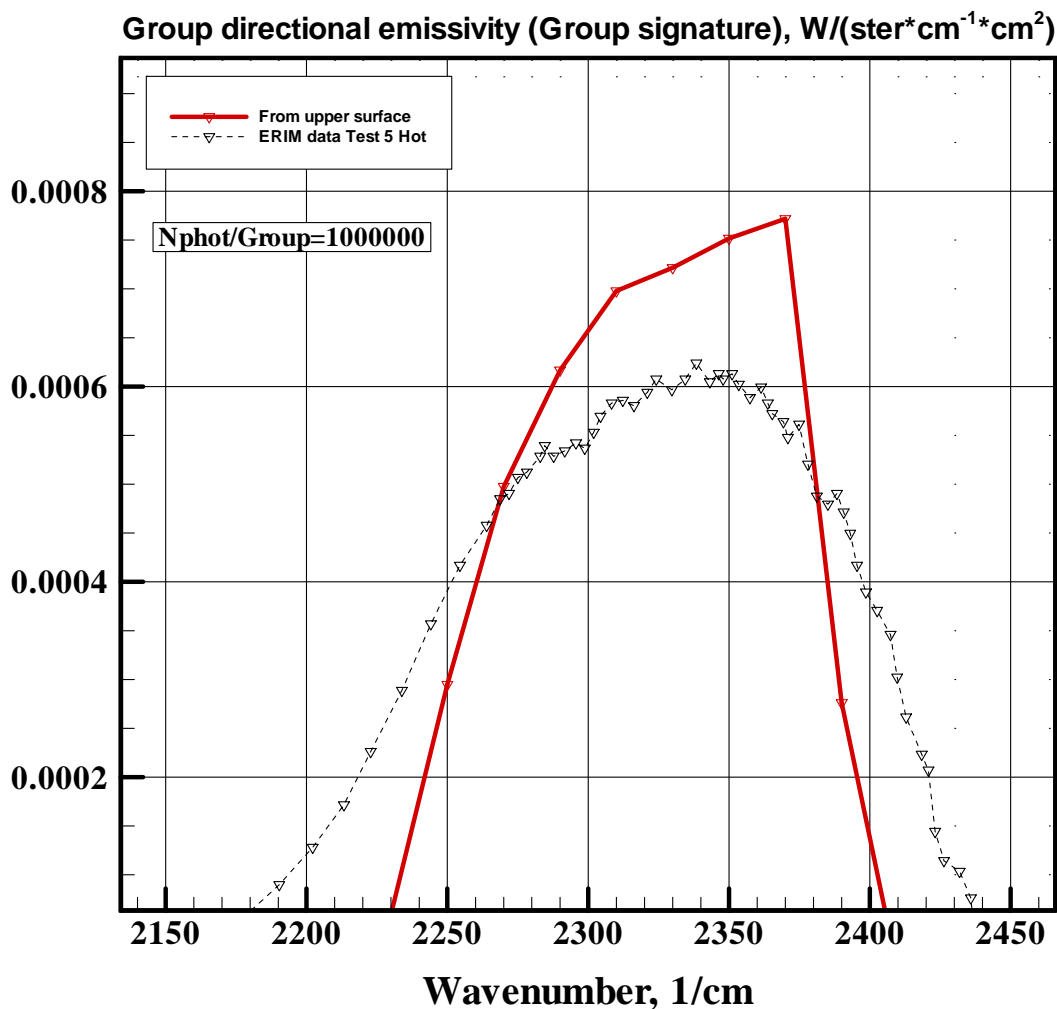


Fig.46. Problem IV. Test 5. ERIM experimental data for CO₂ Hot cell radiance (dotted line) and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The HITRAN temperature-extrapolated data; random model (JLBL=3); spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$

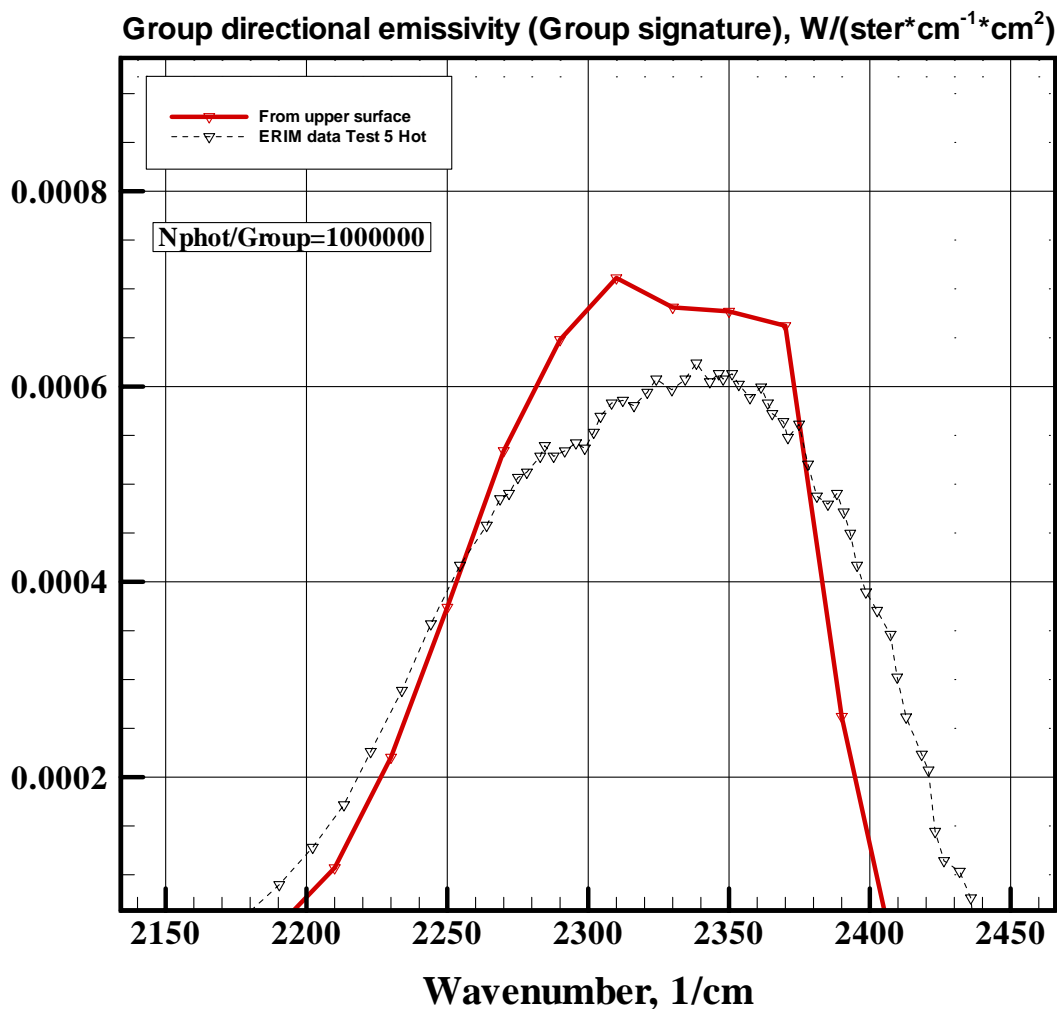


Fig.47. Problem IV. Test 5. ERIM experimental data for CO₂ Hot cell radiance (dotted line) and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The CDSD-1000 data base; averaged rotational line structure (JLBL=0, JSUM=1); spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$

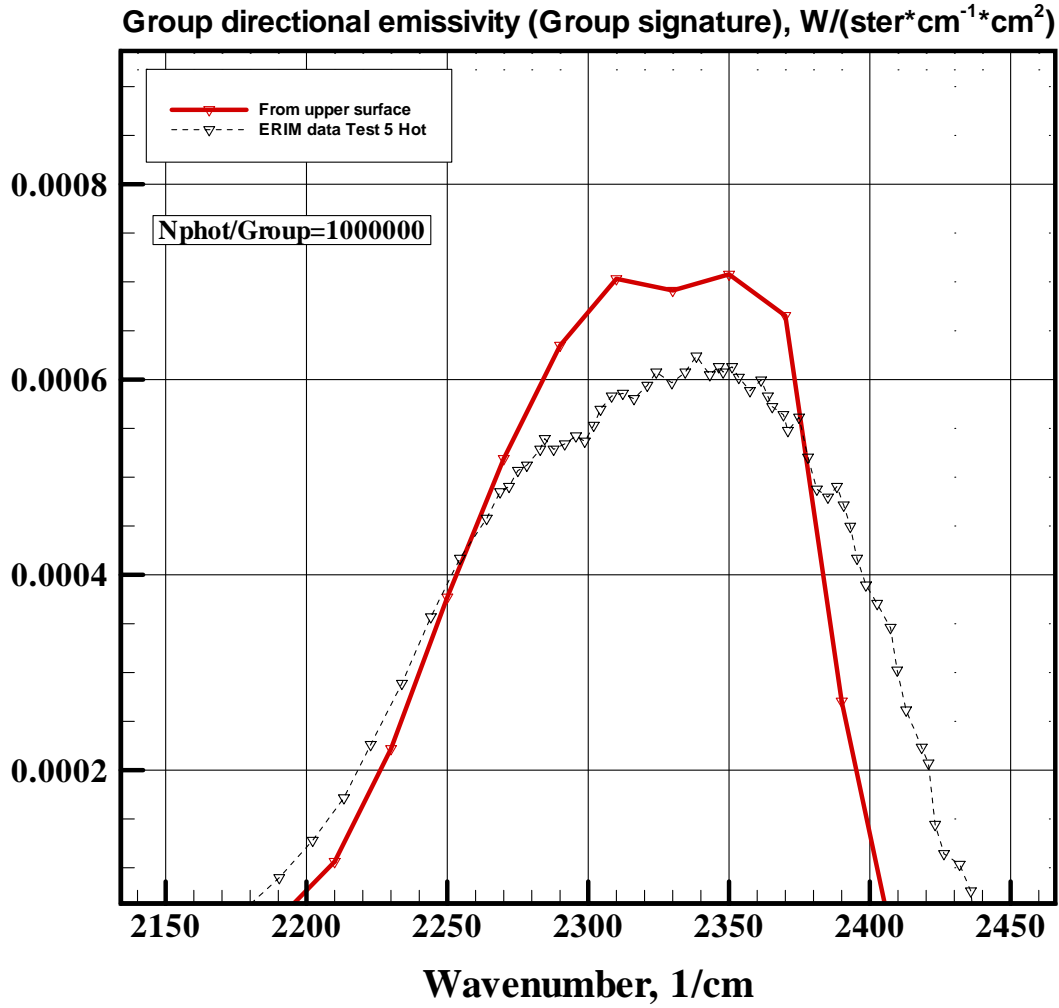


Fig.48. Problem IV. Test 5. ERIM experimental data for CO₂ Hot cell radiance (dotted line) and **Plume-2D-MC** numerical prediction (solid line) of the Hot cell radiance.

The CDSD-1000 data base; random model (JLBL=3); spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$

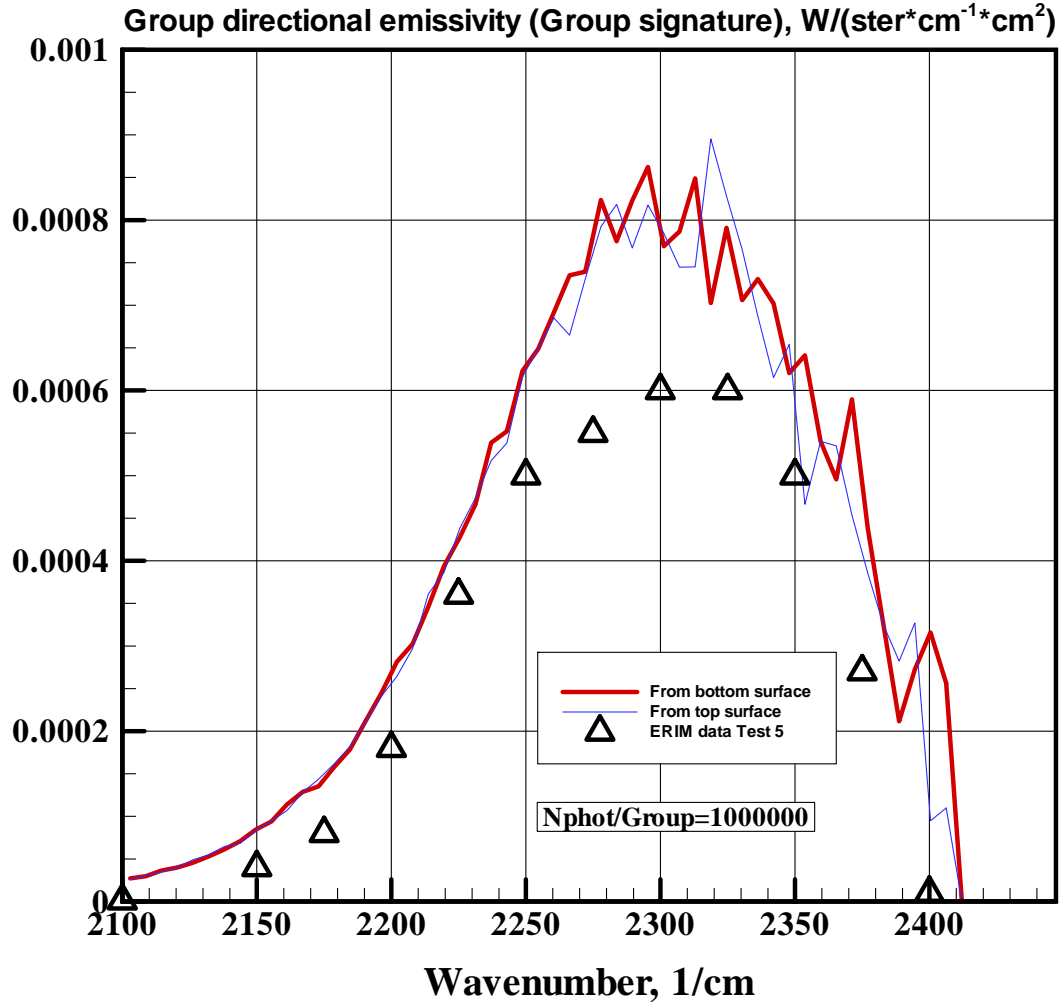


Fig. 49. Problem IV: Spectral signature of homogeneous cylindrical volume heated up to $T = 1200$ K; 2D calculation domain; exponential model [7]; $N_{ph} = 10^6$.
Test 5: CO_2/N_2

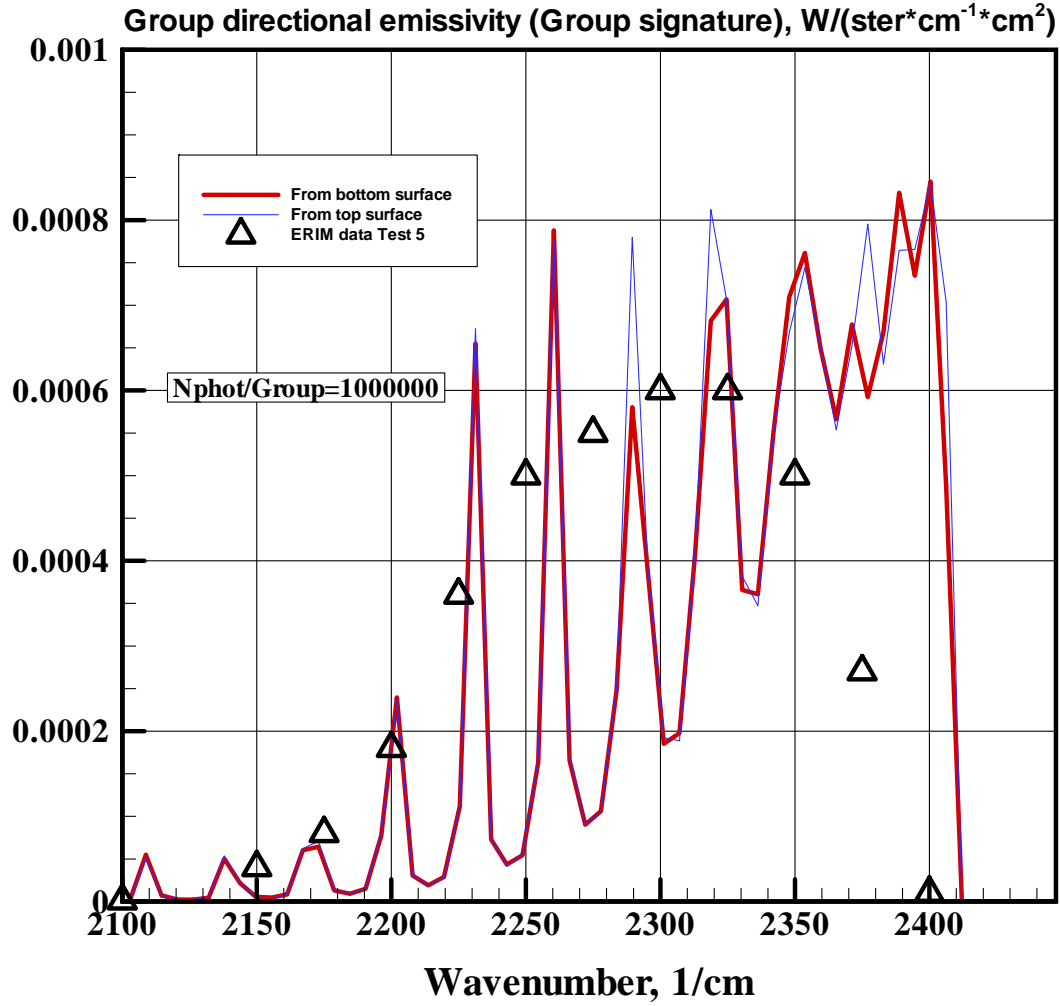


Fig. 50. Problem IV: Spectral signature of homogeneous cylindrical volume heated up to $T=1200$ K; 2D calculation domain; narrow/wide band model [8]; $N_{ph}=10^6$.
Test 5: CO_2/N_2

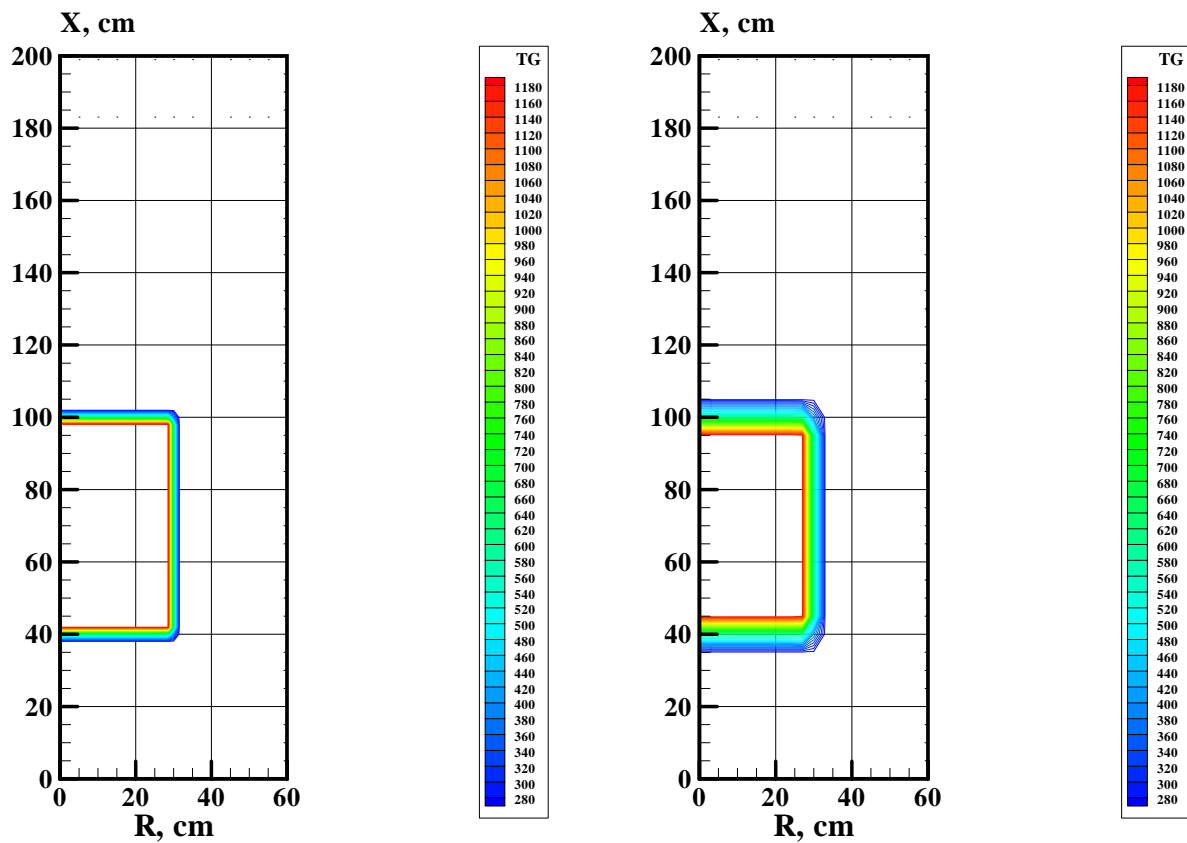


Fig. 51. Schematic of the 2D “Hot/Cold” problem of visibility of heated cylindrical volume of H_2O or CO_2 through cold atmosphere.
Code **Plume_2D_MC**

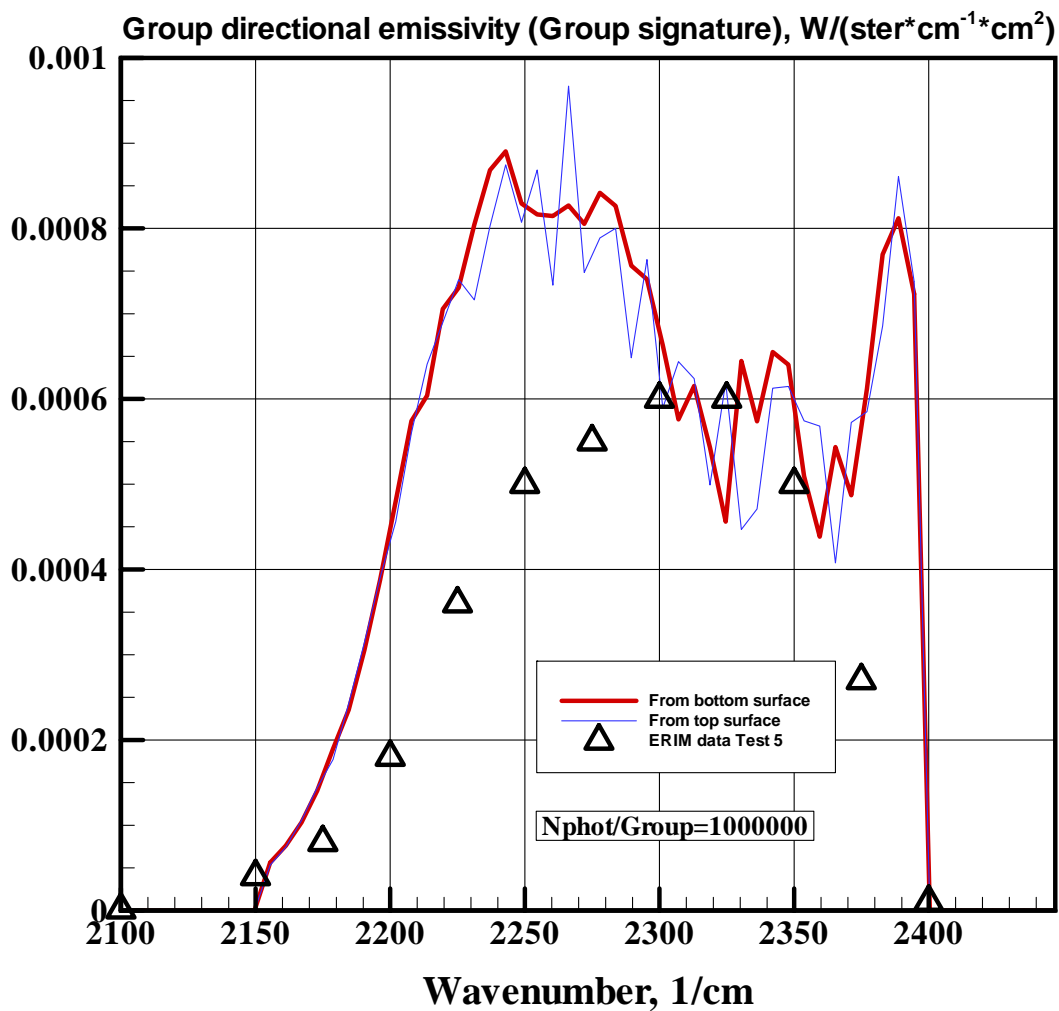


Fig. 52. Problem IV: Spectral signature of homogeneous cylindrical volume heated up to $T = 1200$ K; 2D calculation domain; optical model [3]; $N_{ph} = 10^6$.
Test 5: CO_2/N_2

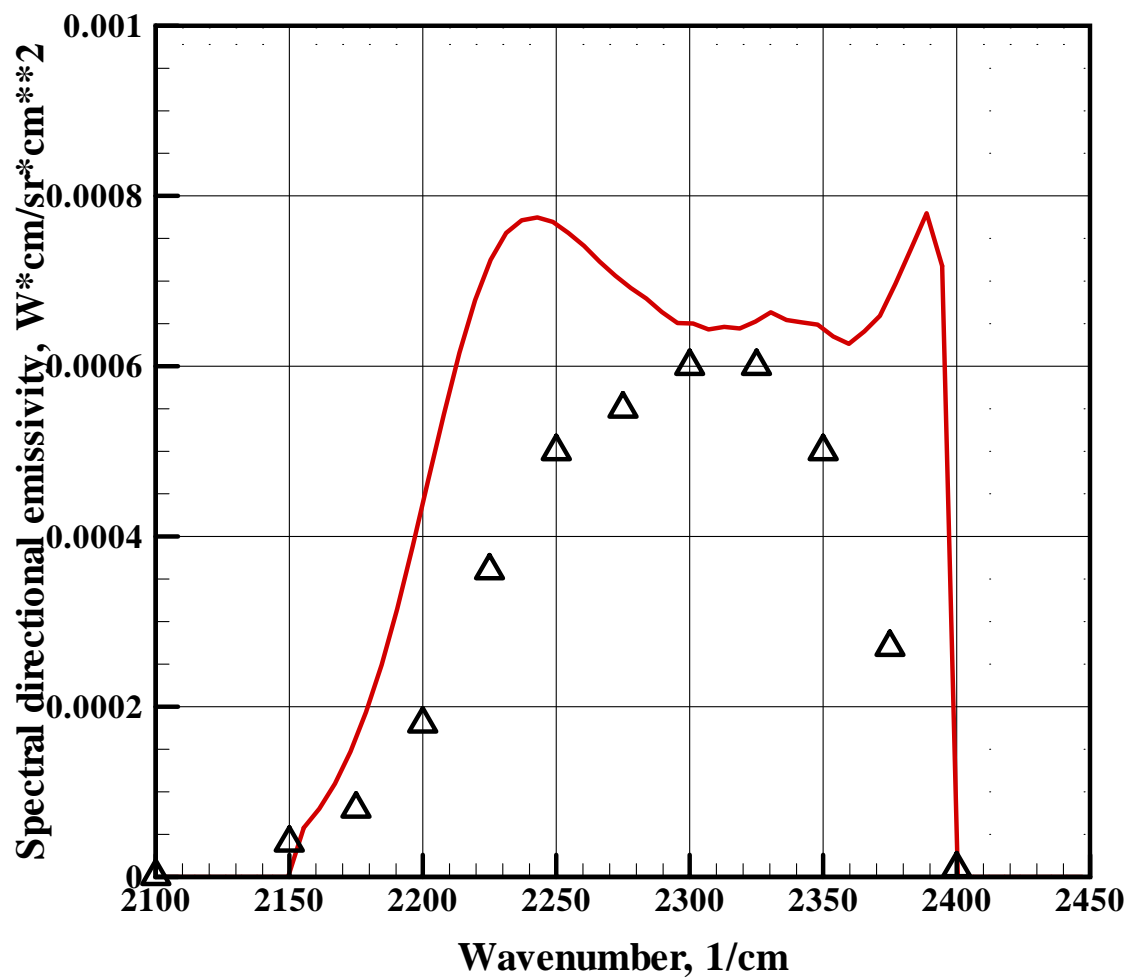


Fig. 53. Problem IV: Spectral signature of homogeneous cylindrical volume heated up to $T=1200$ K; 3D calculation domain; optical model [3]; $N_{ph}=10^4$; the MCLEDE algorithm.
Test 5: CO_2/N_2 .

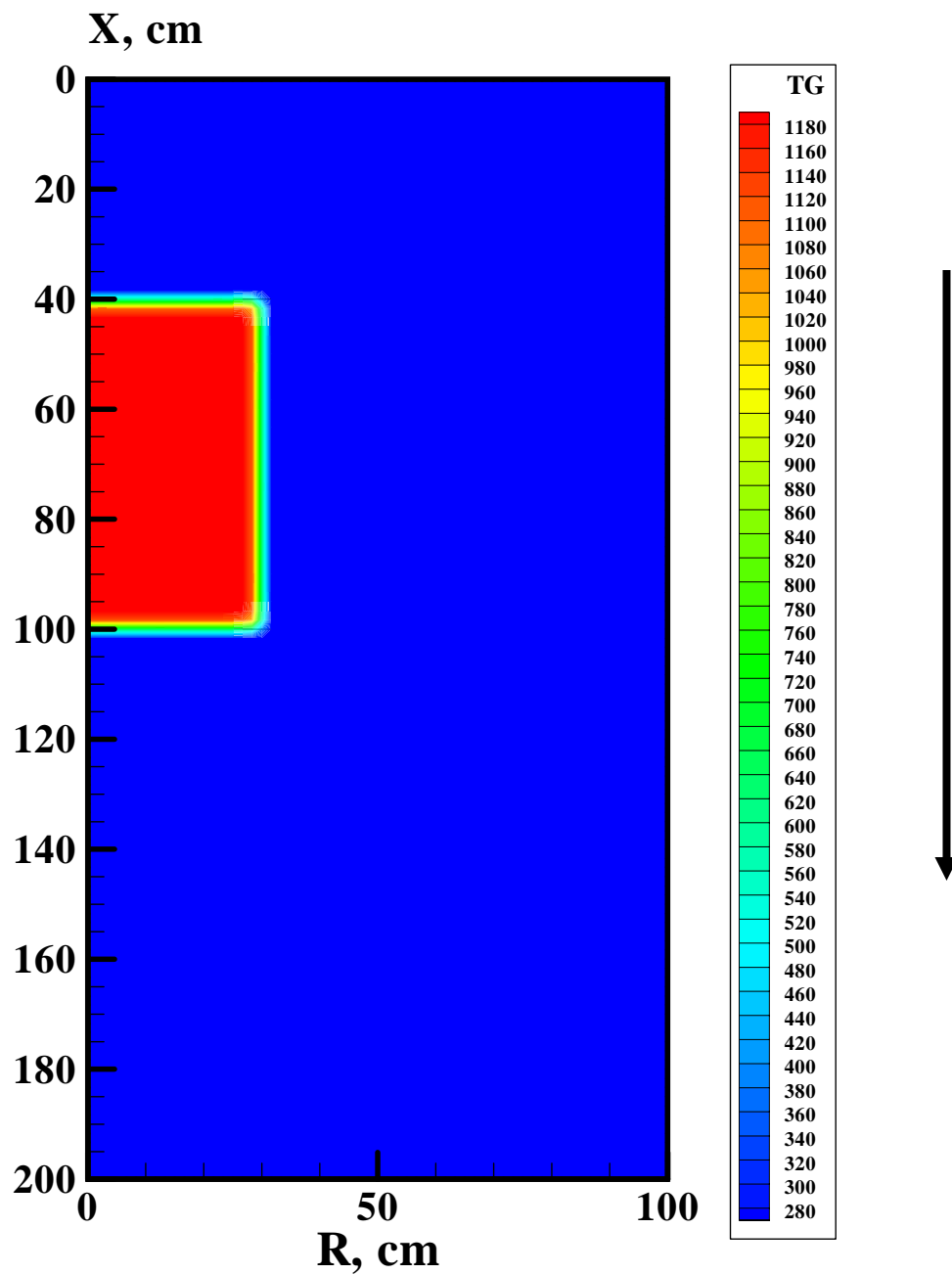


Fig. 54. Problem V: Schematic of 2D “Hot/Cold” problem of visibility of heated cylindrical volume of $\text{H}_2\text{O}/\text{N}_2$ and CO_2/N_2 through cold atmosphere. Code Plume_2D_MC.
Direction of observation is shown by arrow

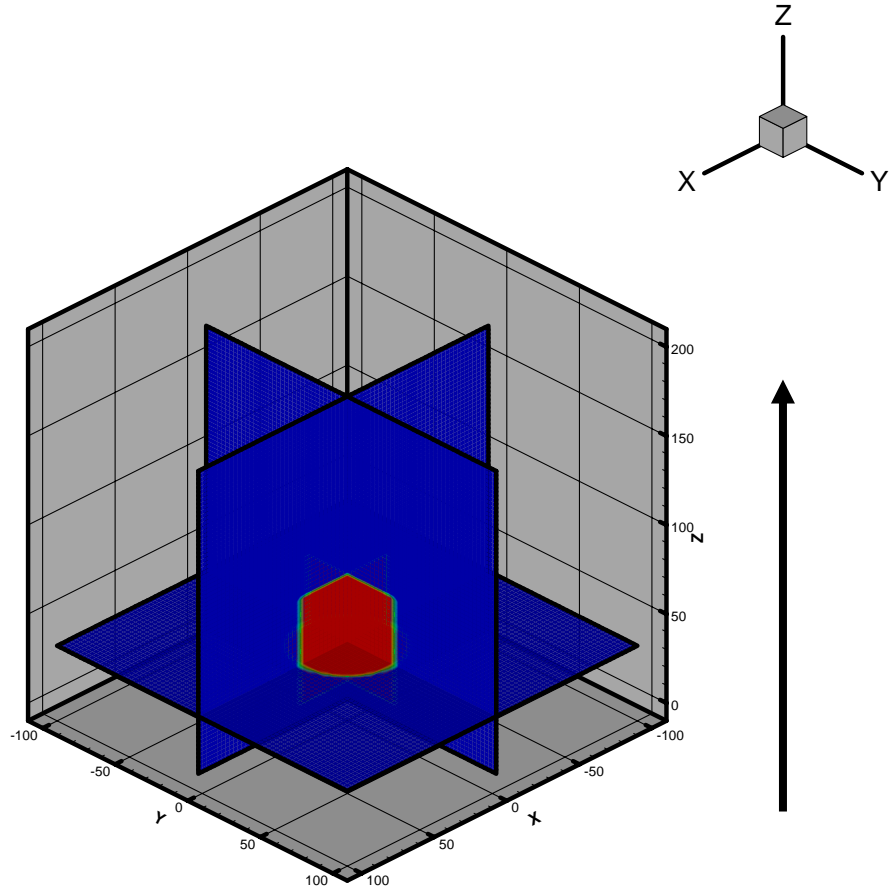


Fig. 55. Problem V: Schematic of 3D “Hot/Cold” problem of visibility of heated cylindrical volume of $\text{H}_2\text{O}/\text{N}_2$ and CO_2/N_2 through cold atmosphere. Code Plume_3D_MC.
Direction of observation is shown by arrow

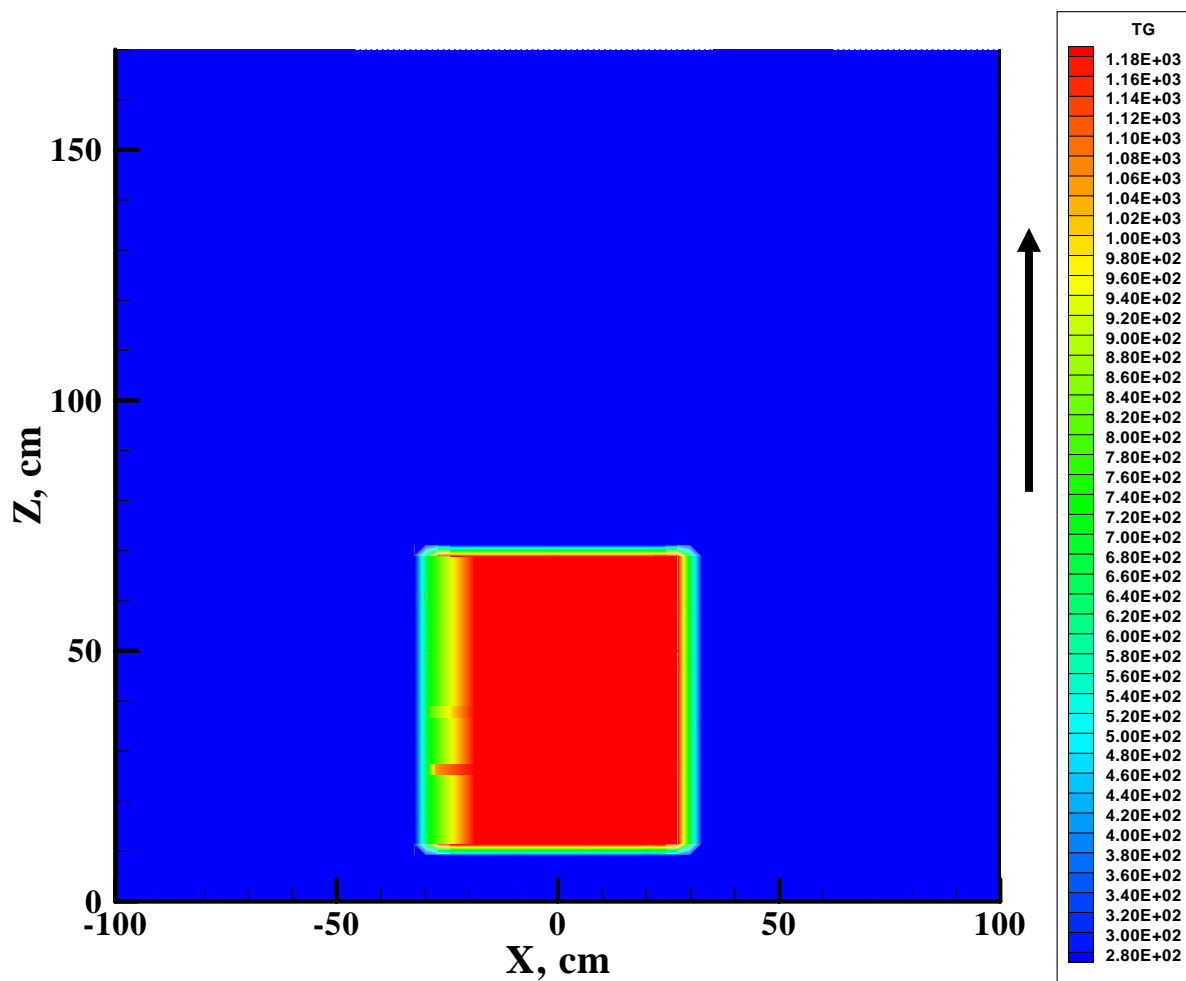


Fig. 56. Problem V: Schematic of 3D “Hot/Cold” problem of visibility of heated cylindrical volume of $\text{H}_2\text{O}/\text{N}_2$ and CO_2/N_2 through cold atmosphere. Code Plume_3D_MC.
Direction of observation is shown by arrow

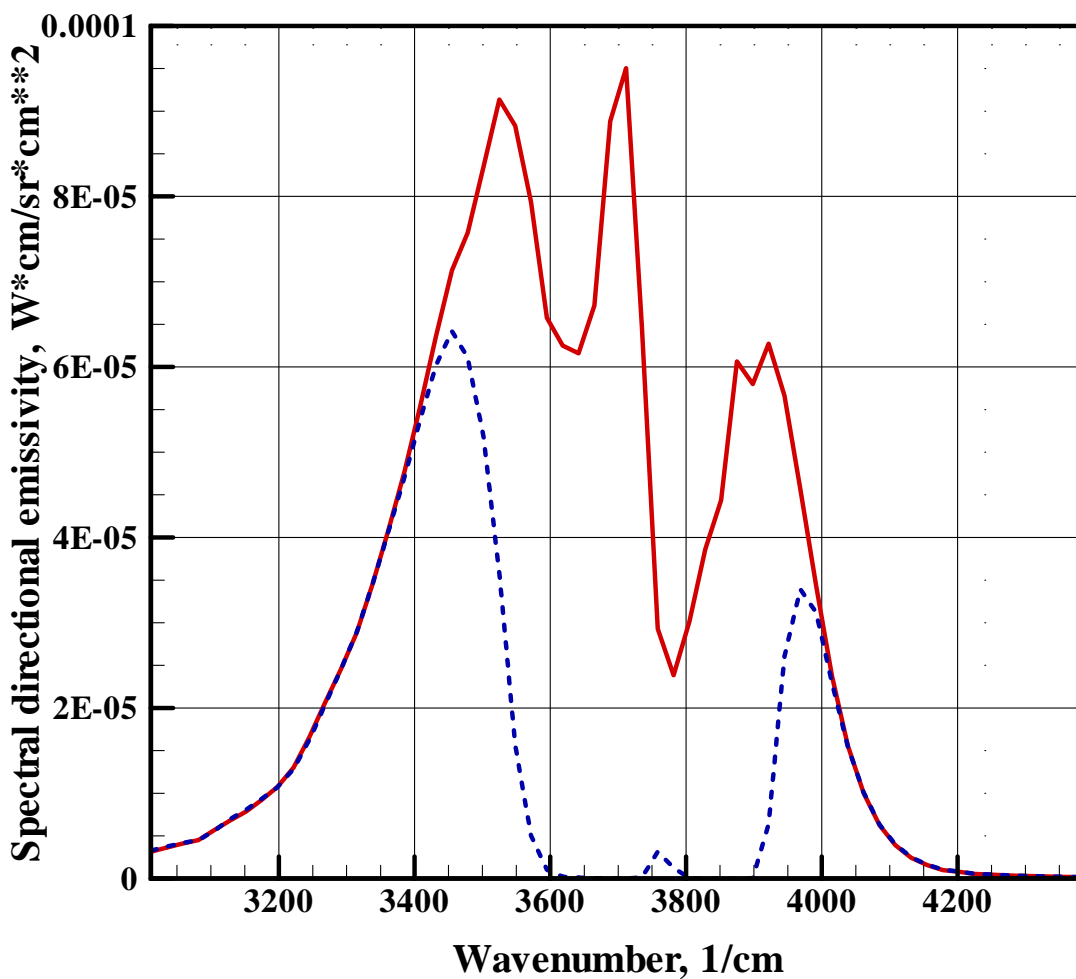


Fig. 57,a. Problem V: Spectral signature of homogeneous cylindrical volume of heated H_2O up to $T=1202\text{ K}$; 3D calculation domain; $N_{ph}=10^4$; the MCLEDE algorithm. Solid line- prediction of Hot cell radiance (Test 9R); dotted line – prediction of Hot-through-Cold cell radiance (Test-9R).
The NASA standard infrared model of averaged rotational lines structure

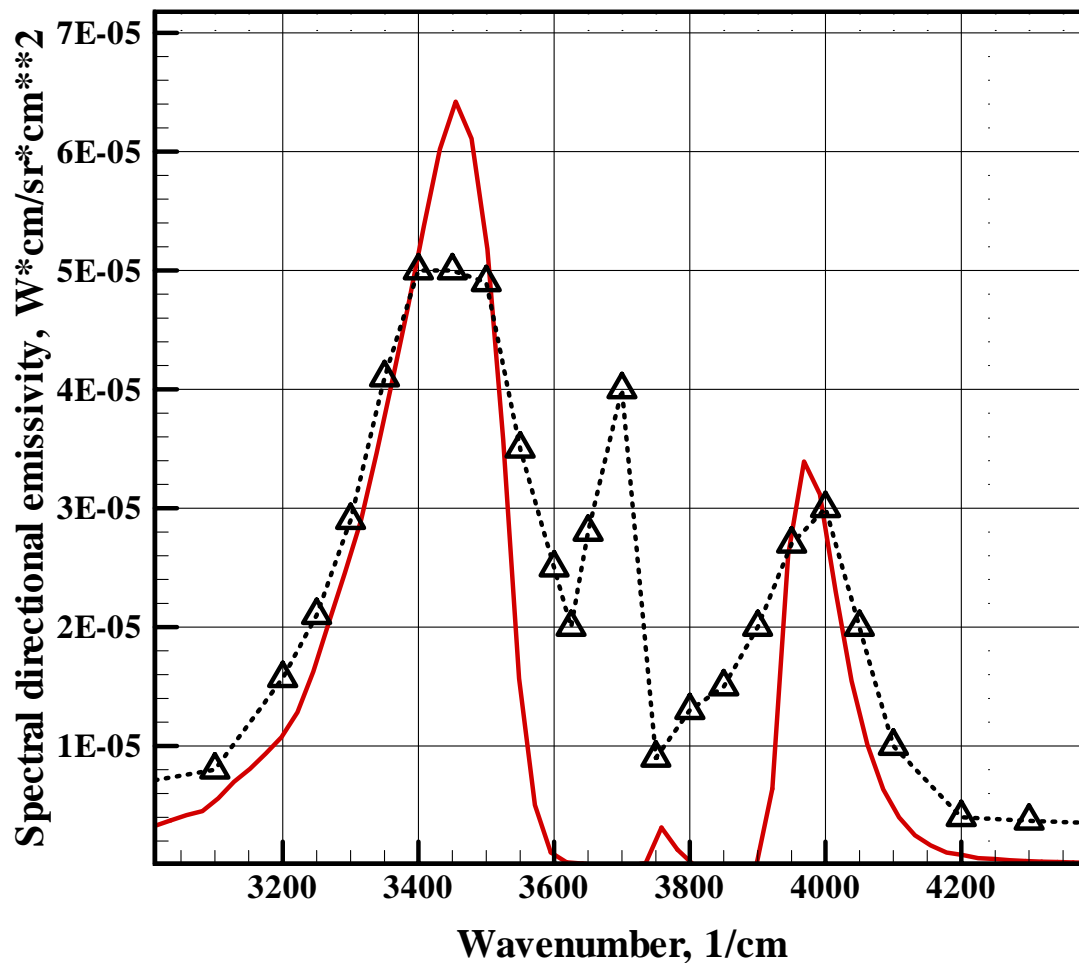


Fig. 57,b. Problem V: Spectral signature of homogeneous cylindrical volume of heated H₂O up to T=1202 K; 3D calculation domain; $N_{ph} = 10^4$; the MCLEDE algorithm. Code Plume-3D-MC.
Solid line – prediction of Hot-through-Cold cell radiance,
Dotted line – ERIM experimental points for Test-9R

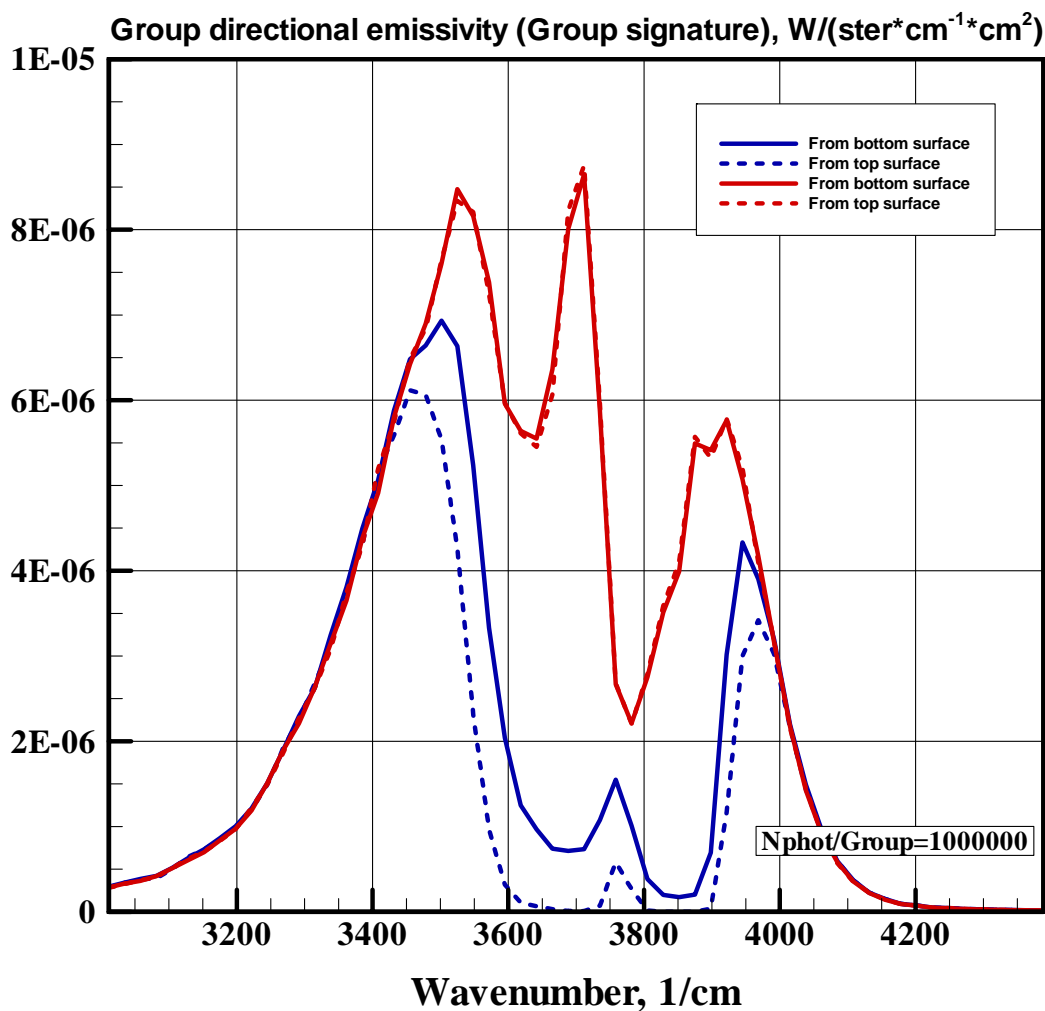


Fig. 58. Problem V: Spectral signature of homogeneous cylindrical volume of heated H_2O up to $T=1202$ K; 2D calculation domain; $N_{ph}=10^6$. Code Plume_2D_MC.
 Upper lines – prediction of Hot cell radiance (Test-9R);
 Lower lines – prediction of Hot-through-cold radiance (Test-9R)

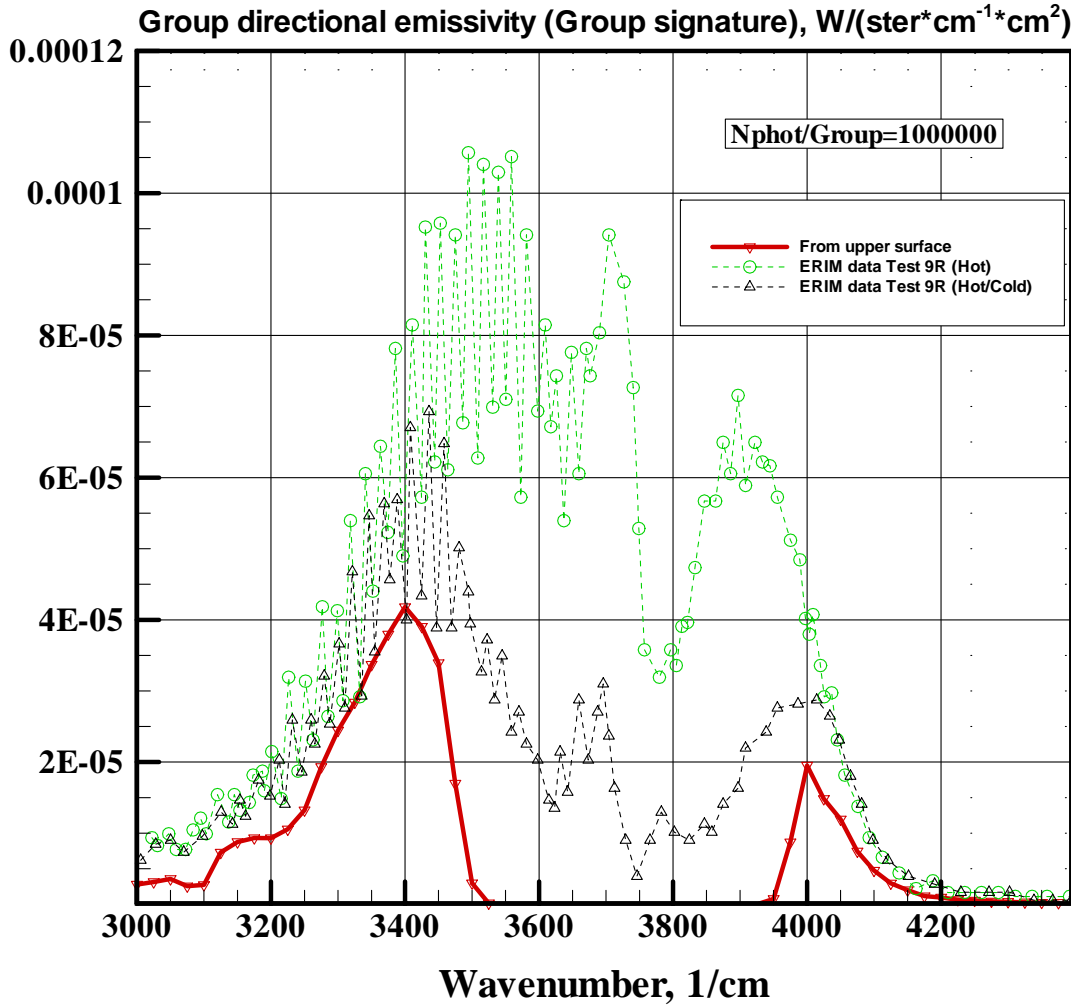


Fig.59. Problem V. Test 9R. ERIM experimental data for H₂O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot –through-cold radiance.

The NASA standard infrared radiation model; random model (JLBL=2); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

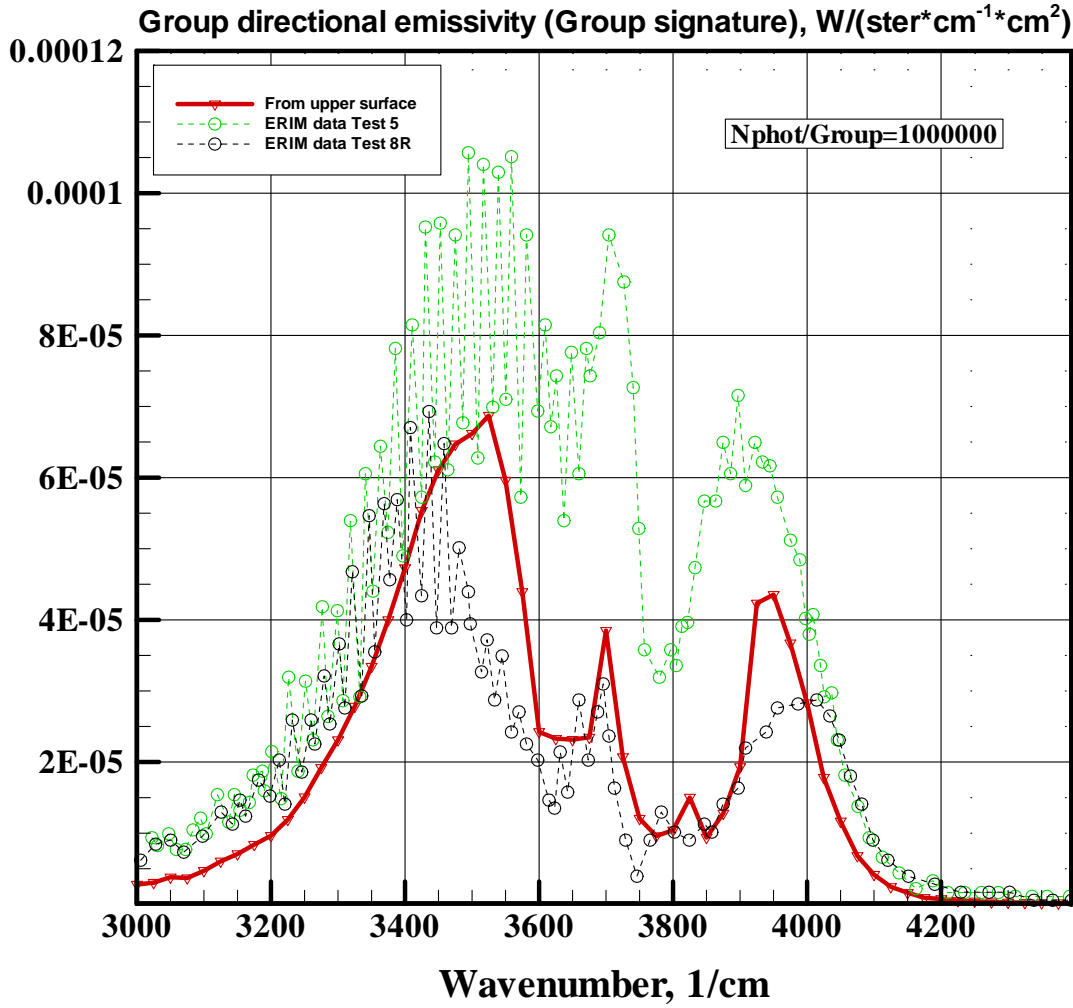


Fig. 60. Problem V. Test 9R. ERIM experimental data for H₂O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot –through-cold radiance.

The NASA standard infrared radiation model; random model (JLBL=2); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

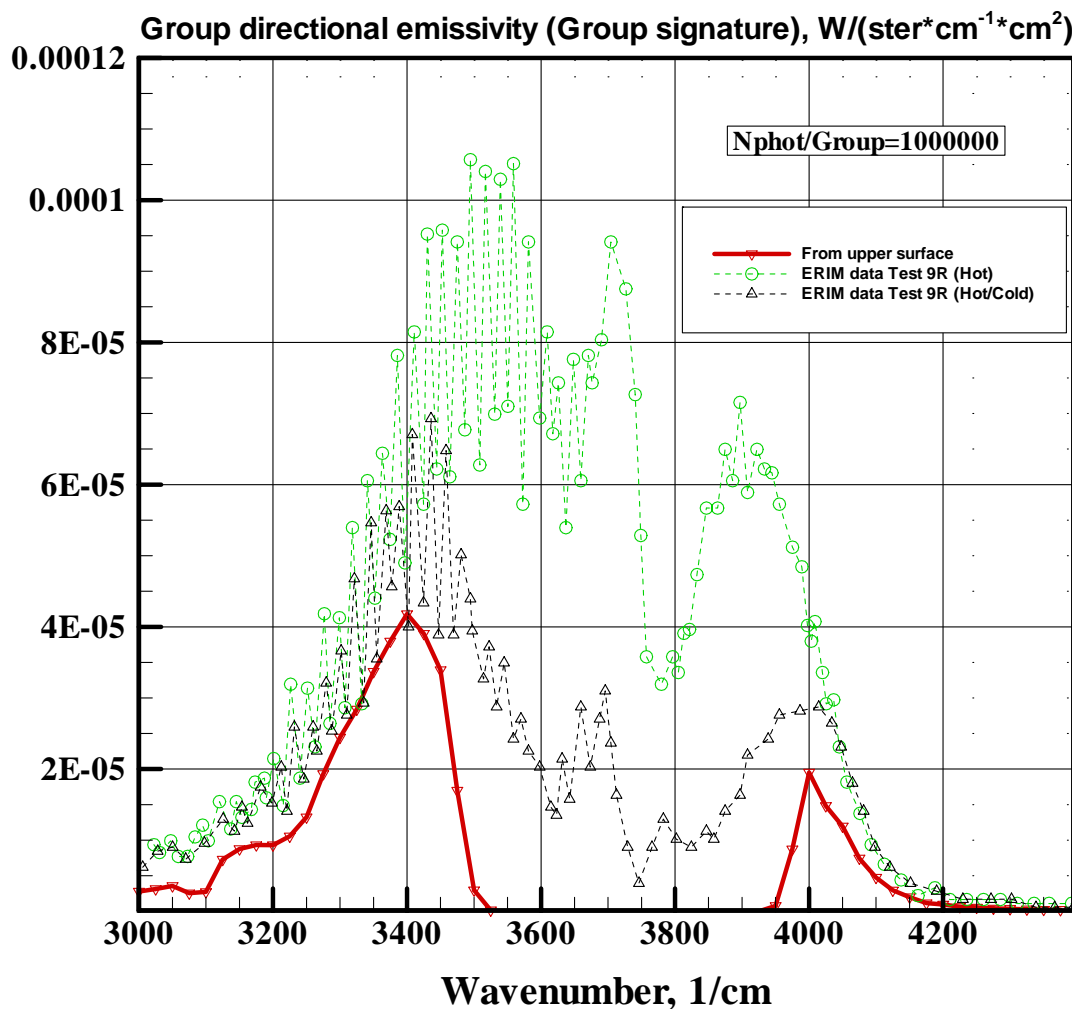


Fig.61. Problem V. Test 9R. ERIM experimental data for H₂O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot-through-Cold radiance.

The HITRAN temperature-extrapolated data; averaged rotational line structure (JLBL=0); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

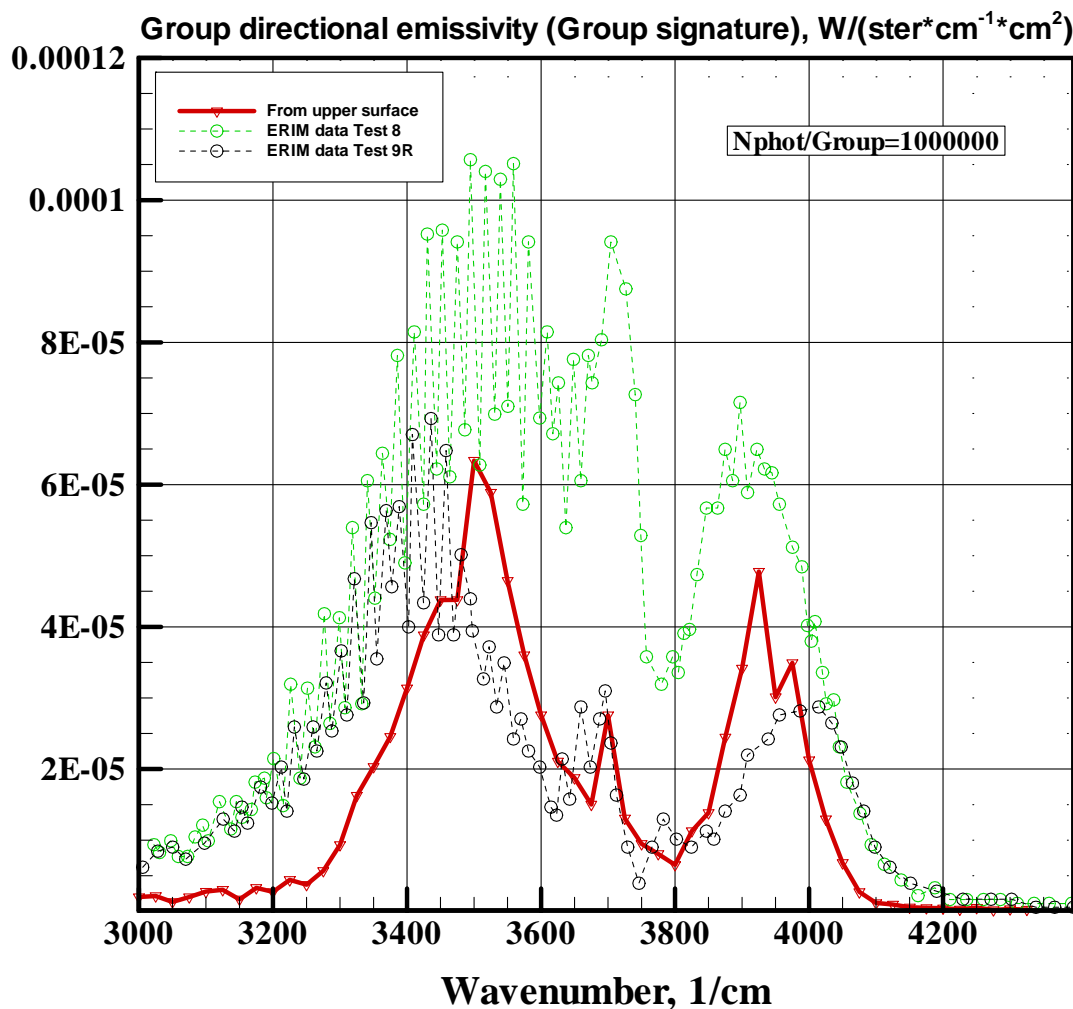


Fig.62. Problem V. Test 9R. ERIM experimental data for H₂O Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot-through-Cold radiance.

The HITRAN temperature-extrapolated data; averaged rotational line structure (JLBL=3); spectral region for each spectral group is $\Delta\omega = 25 \text{ cm}^{-1}$

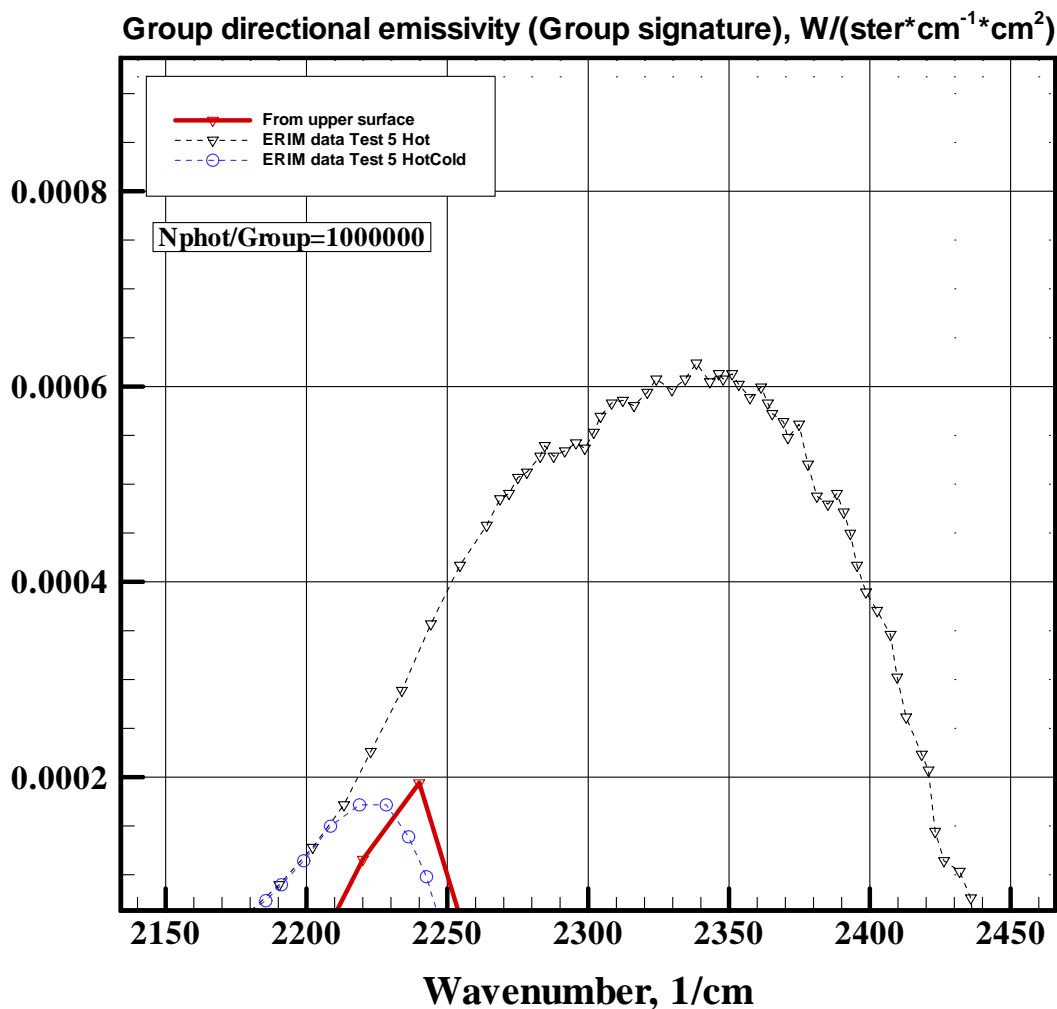


Fig.63. Problem V. Test 5. ERIM experimental data for CO₂ Hot cell radiance (upper dotted line), Hot-through-cold radiance (lower dotted line), and **Plume-2D-MC** numerical prediction (solid line) of the Hot-through-Cold radiance.

The HITRAN temperature-extrapolated data; random model (JLBL=3); spectral region for each spectral group is $\Delta\omega = 20 \text{ cm}^{-1}$

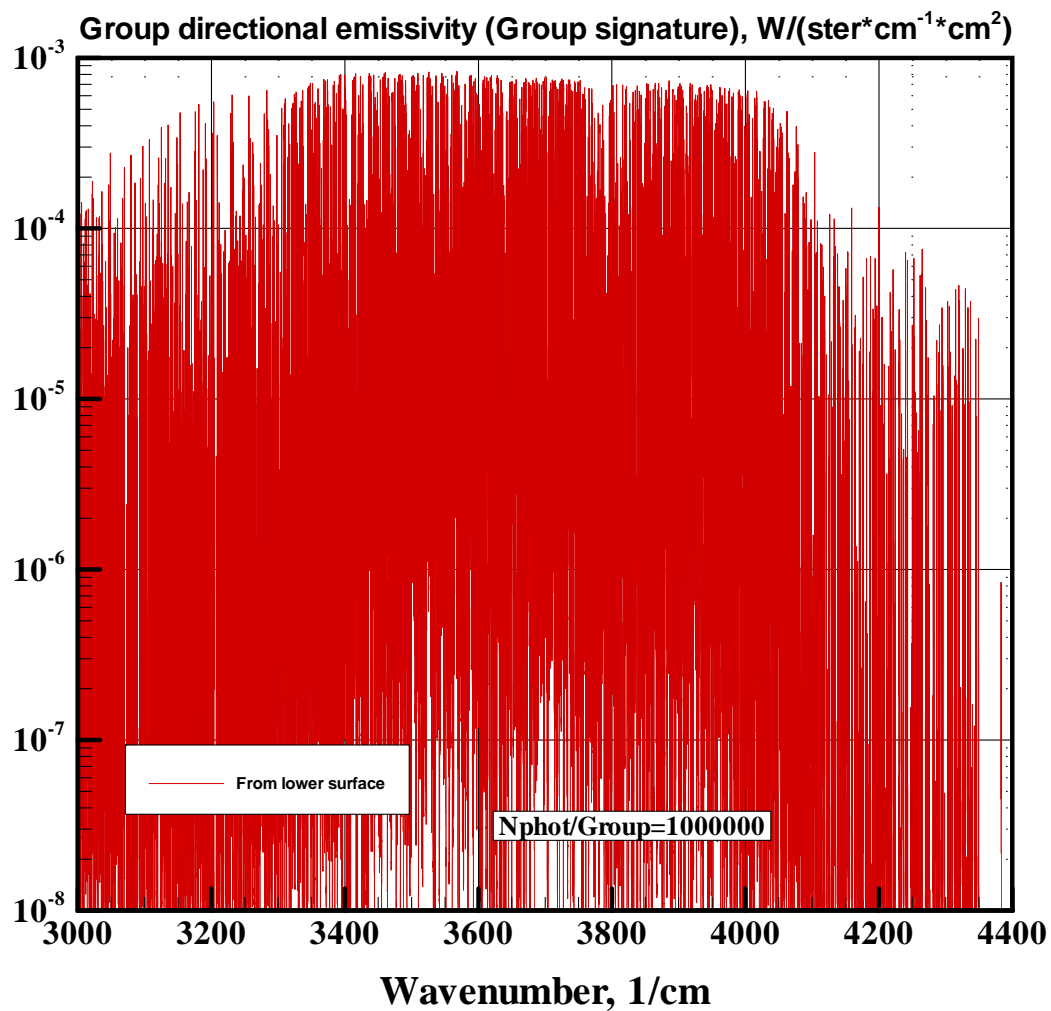


Fig. 64,a. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot cell $\text{H}_2\text{O}/\text{N}_2$ radiance; spectral resolution is $\Delta\omega=0.0083 \text{ cm}^{-1}$

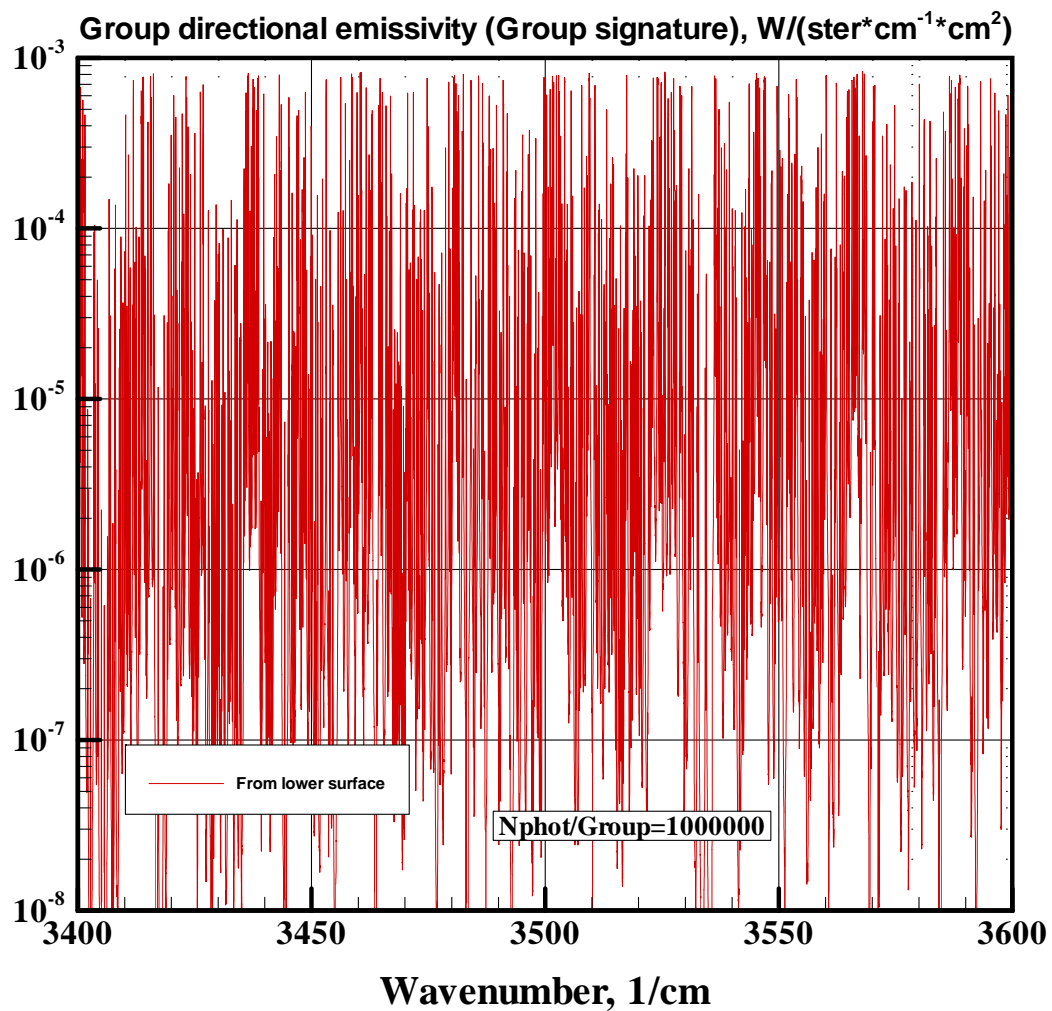


Fig. 64,b. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot cell $\text{H}_2\text{O}/\text{N}_2$ radiance; spectral resolution is $\Delta\omega = 0.0083 \text{ cm}^{-1}$

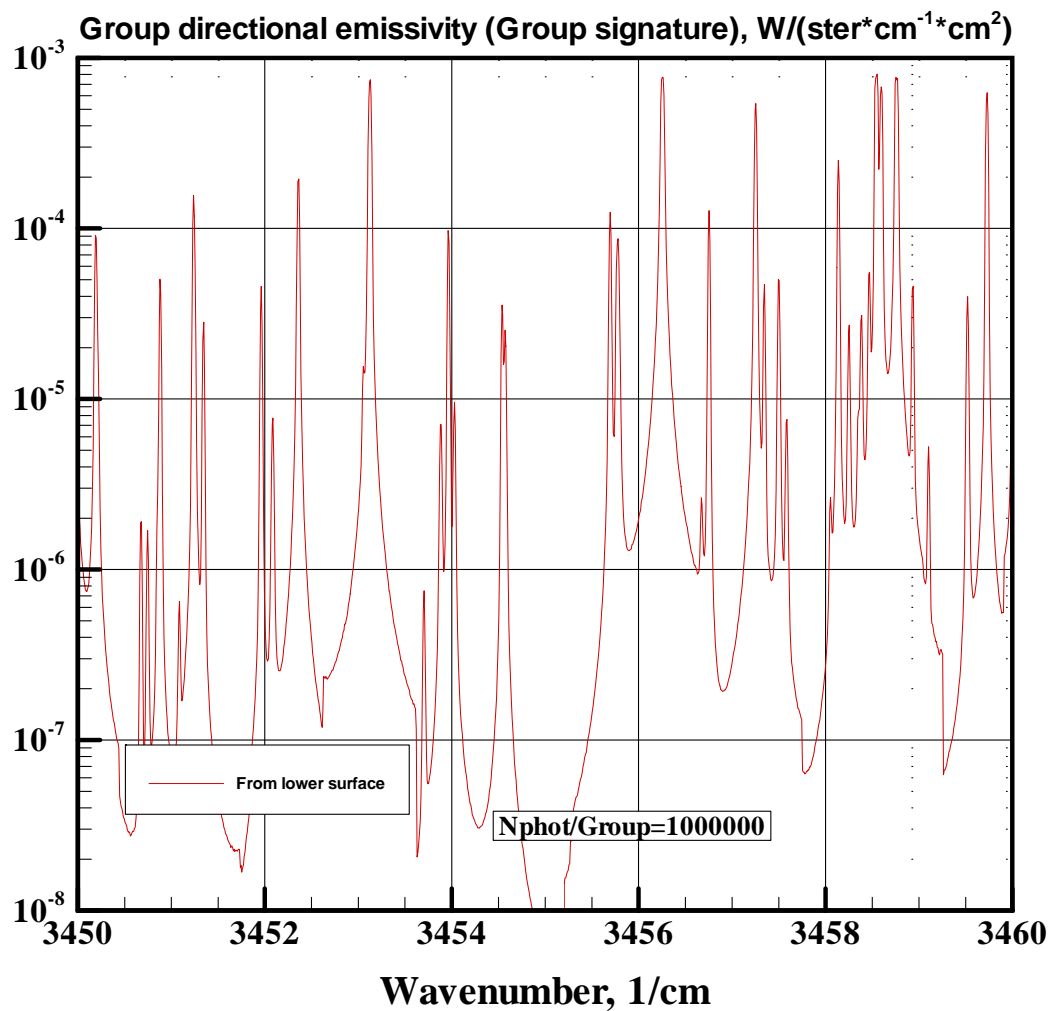


Fig. 64,c. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot cell $\text{H}_2\text{O}/\text{N}_2$ radiance; spectral resolution is $\Delta\omega = 0.0083 \text{ cm}^{-1}$

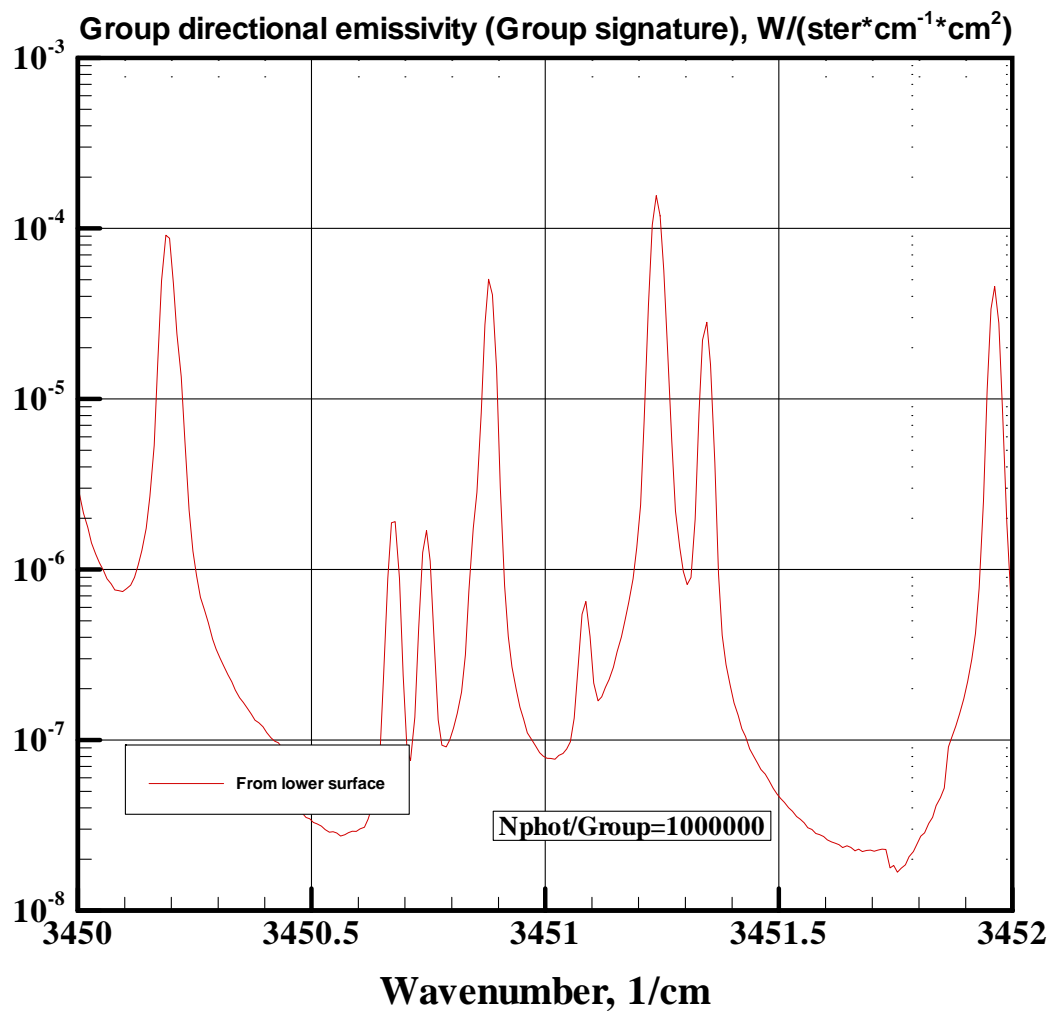


Fig. 64,d. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot cell $\text{H}_2\text{O}/\text{N}_2$ radiance; spectral resolution is $\Delta\omega = 0.0083 \text{ cm}^{-1}$

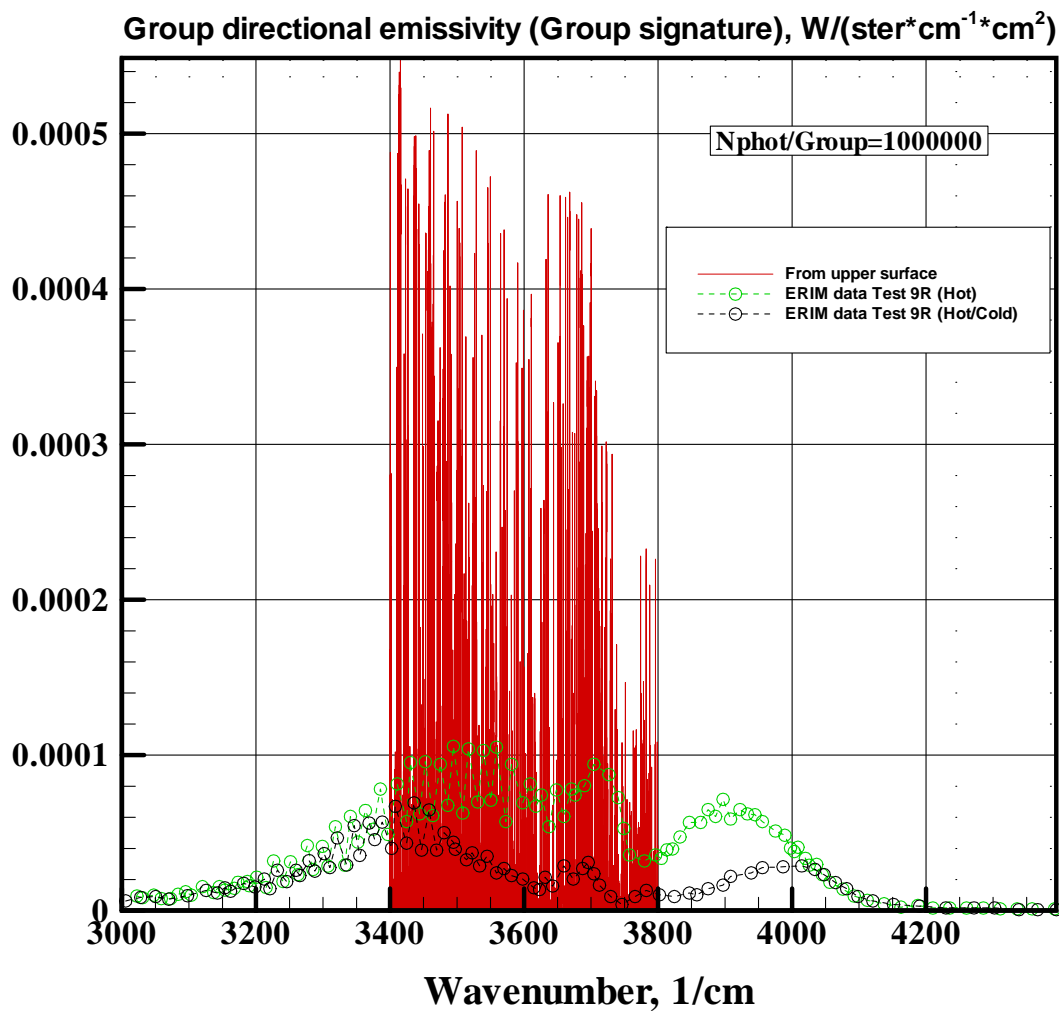


Fig. 65,a. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot-through-cold radiance ($\text{H}_2\text{O}/\text{N}_2$); spectral resolution is $\Delta\omega = 0.0083 \text{ cm}^{-1}$

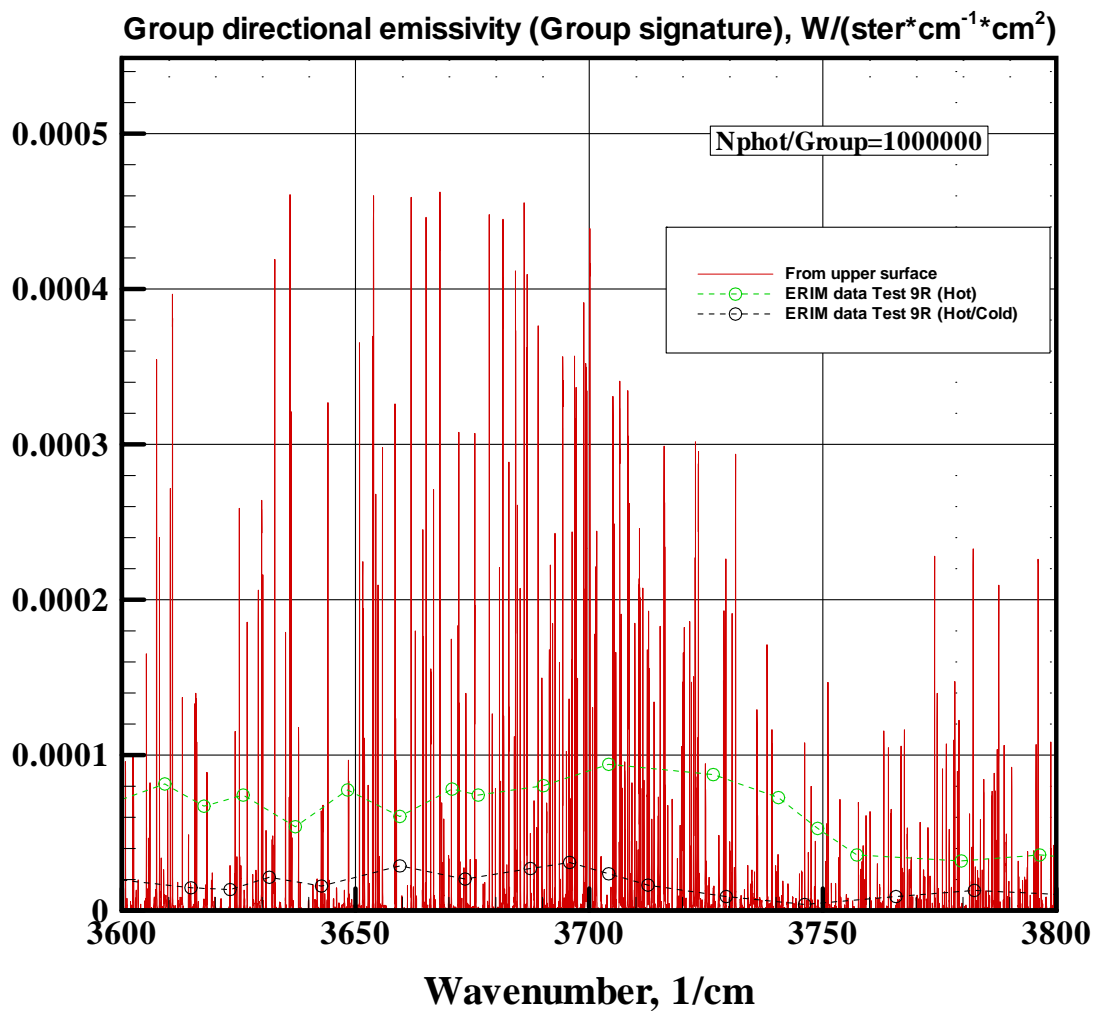


Fig. 65,b. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot-through-cold radiance ($\text{H}_2\text{O}/\text{N}_2$); spectral resolution is $\Delta\omega = 0.0083 \text{ cm}^{-1}$

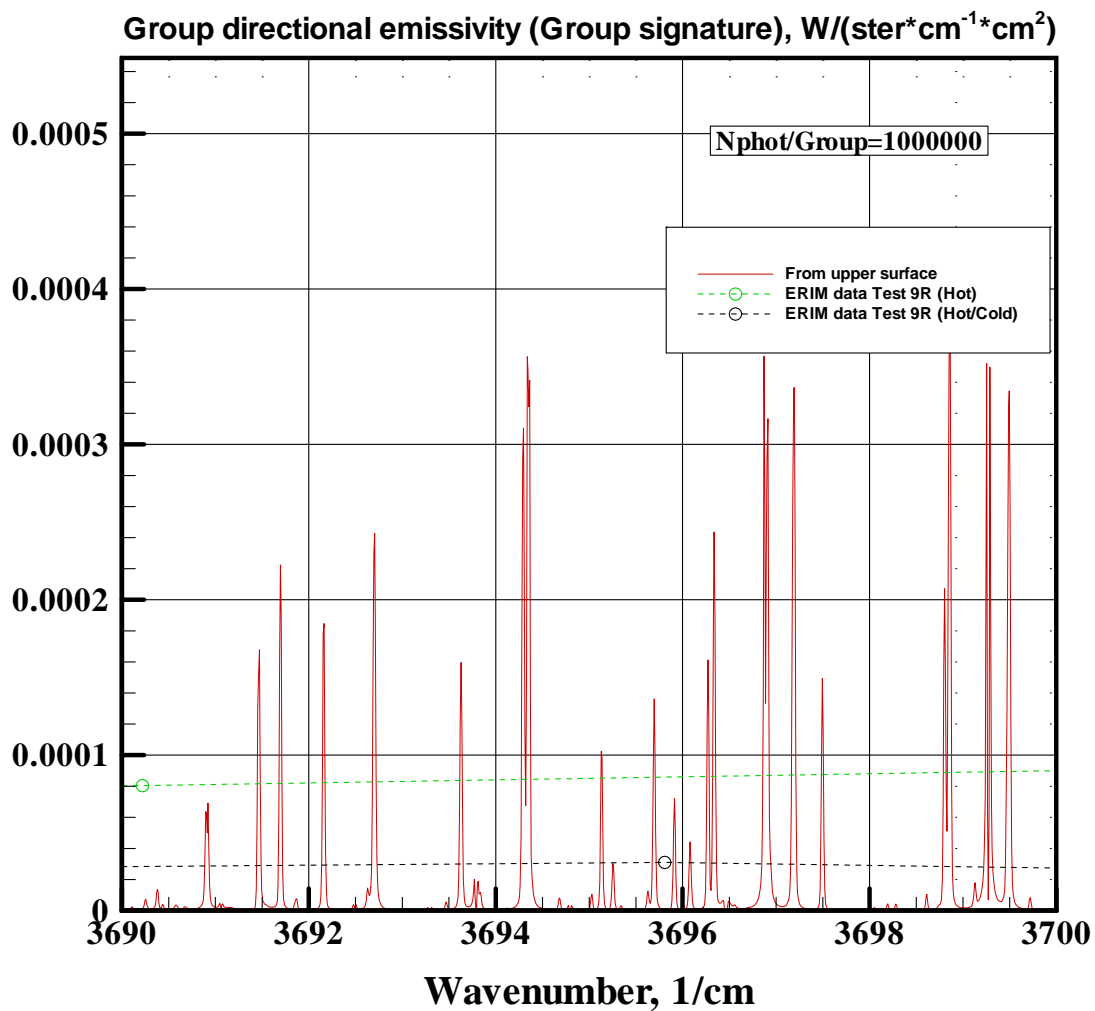


Fig. 65,c. Line-by-line prediction of spectral intensity for conditions of ERIM experiments (Test 9R); Hot-through-cold radiance ($\text{H}_2\text{O}/\text{N}_2$); spectral resolution is $\Delta\omega = 0.0083 \text{ cm}^{-1}$

Code **PLUME-2D-MC**
Functional arrangement

MC_Plumes.FOR				Main program
	SUBROUTINE InFields			Generation of spatial distributions for gasdynamic functions: <ul style="list-style-type: none"> - gas temperature, - and solid particles temperatures, - pressure, - molar fractions of gas species (x_i), - concentration of solid particles (n_i)
		SUBROUTINE TECPLOT_GD_Fields		Graphical representation of gasdynamic functions
	SUBROUTINE GenCodeMC			<ol style="list-style-type: none"> 1. Preparation of spectral (group) optical properties for Monte-Carlo simulation 2. Loop organization of Monte-Carlo simulation on spectral groups. 3. Final representation of calculated data
		SUBROUTINE INPDD		Initial conditions input: <ol style="list-style-type: none"> 1. Initial conditions for Monte-Carlo simulation 2. Initial conditions for optical models
			SUBROUTINE CONVERT_DISK_RAM_ HITRAN	Reading data from Data Base HITRAN into RAM
			SUBROUTINE CONVERT_DISK_RAM_ CSDS_1000	Reading data from Data Base CSDS-1000 into RAM
		SUBROUTINE INPROP		Gasdynamic functions distributions reading into RAM
		SUBROUTINE OPTICS		Calculation of spectral (group) optical properties of gaseous species for given thermodynamic point (ω , T , p , x_i)
		SUBROUTINE SOLAB		Calculation of spectral (group) optical properties of solid particles for given thermodynamic point (ω , T^p , n_i)
		SUBROUTINE SCAIN		Calculation of spectral (group) phase function of scattering of solid particles for given thermodynamic point (ω , T^p , n_i). The Henyey – Greenstein scattering indicatrix
		SUBROUTINE		Calculation of spectral (group) phase function of

Monte-Carlo Simulation of Plumes Spectral Emission

		SCAIR		scattering of solid particles for given thermodynamic point (ω , T^p , n_i). The Henyey – Greenstein scattering indicatrix
		SUBROUTINE PROB_Simple		Monte-Carlo simulation without taking into account of rotational line structure (JLBL=0,1)
		SUBROUTINE PROB_Hybrid		Monte-Carlo simulation with taking into account of rotational line structure (JLBL=2,3)

SUBROUTINE OPTICS.

Functional arrangement

SUBROUTINE OPTICS				Calculation of spectral (group) optical properties of gaseous species for given thermodynamic point (ω , T , p , x_i)
	SUBROUTINE LBL_Absorption_Coefficient			Line-by-Line calculation of spectral (group) optical properties of gaseous species for given thermodynamic point (ω , T , p , x_i). These calculations are based on HITRAN-like databases
	SUBROUTINE ABS_EMPIRICAL			Calculation of spectral (group) optical properties of gaseous species for given thermodynamic point (ω , T , p , x_i). These calculations are based on semi-empirical NASA standard infrared model of averaged rotational line structure
		SUBROUTINE H2O_EMPIR		Prediction of averaged absorption coefficient (S/d) and lines density ($1/d$) for H ₂ O.
			FUNCTION BILINT	Two-dimensional interpolation
		SUBROUTINE CO2_EMPIR		Prediction of averaged absorption coefficient (S/d) and lines density ($1/d$) for CO ₂ .
			FUNCTION BILINT	Two-dimensional interpolation
		SUBROUTINE CO_EMPIR		Prediction of averaged absorption coefficient (S/d) and lines density ($1/d$) for CO.
			FUNCTION BILINT	Two-dimensional interpolation
		SUBROUTINE HCL_EMPIR		Prediction of averaged absorption coefficient (S/d) and lines density ($1/d$) for HCl.
			FUNCTION BILINT	Two-dimensional interpolation
		SUBROUTINE HF_EMPIR		Prediction of averaged absorption coefficient (S/d) and lines density ($1/d$) for HF.
			FUNCTION BILINT	Two-dimensional interpolation
	SUBROUTINE ABS_EXP_MOD			Calculation of spectral (group) optical properties of gaseous species for given thermodynamic point (ω , T , p , x_i). These calculations are based on semi-analytical wide-band exponential models of averaged rotational line structure.

		SUBROUTINE H2OEXP_M		Prediction of averaged absorption coefficient (S/d) and lines density (l/d) for H ₂ O.
			FUNCTION FVVV	
		SUBROUTINE CO2EXP_M		Prediction of averaged absorption coefficient (S/d) and lines density (l/d) for CO ₂ .
			FUNCTION F1 FUNCTION F2 FUNCTION F3	
	SUBROUTINE ABS_TONG			Calculation of spectral (group) optical properties of gaseous species for given thermodynamic point (ω , T , p , x_i). These calculations are based on semi-analytical wide/narrow-band exponential models of averaged rotational line structure [Li W., Tong T.W., Dobranich D., Gritz L.A. "A Combined Narrow- and Wide-Band Model for Computing the Spectral Absorption Coefficient of CO ₂ , CO, H ₂ O, CH ₄ , C ₂ H ₂ , and NO", JQSRT, 1995, Vol. 54, No. 6, pp. 961–970].
		SUBROUTINE gasp1_0		
			SUBROUTINE CO2	
			SUBROUTINE H2O	
			SUBROUTINE CO	
			SUBROUTINE CH4	
			SUBROUTINE C2H2	
			SUBROUTINE NO	

SUBROUTINE SOLAB
Functional arrangement

SUBROUTINE SOLAB			Calculation of spectral (group) optical properties of solid particles for given thermodynamic point (ω , T^p , n_i)
	SUBROUTINE H2OL		Prediction of spectral optical properties of liquid particles of H ₂ O: absorption coefficient, scattering coefficient
		SUBROUTINE MIEC	Calculation of spectral optical properties of dielectric sphere by the Mie theory
	SUBROUTINE AL2O3		Prediction of spectral optical properties of solid particles of Al ₂ O ₃ : absorption coefficient, scattering coefficient
		SUBROUTINE MIEC	Calculation of spectral optical properties of dielectric sphere by the Mie theory
	SUBROUTINE SOOT		Prediction of spectral optical properties of solid particles of soot (C): absorption coefficient, scattering coefficient
		SUBROUTINE MIEC	Calculation of spectral optical properties of dielectric sphere by the Mie theory

SUBROUTINE PROBT_Simple
Functional arrangement

SUBROUTINE PROBT_Simple			Monte-Carlo simulation without taking into account of rotational line structure (JLBL=0,1)
	SUBROUTINE MEAN		Averaging of temperatures (gas and solid/liquid phases) and optical properties inside elementary calculation zones (volumes)
		FUNCTION SUMAM	Integration of any function
	SUBROUTINE EXPELL		Prediction of volume emission of each elementary calculation volume
		FUNCTION BlackBodyFunction	Calculation of the Planck function for given parameters ω and T
	SUBROUTINE INCOOR		Prediction of initial spatial coordinate for each photon
		SUBROUTINE FI	Prediction of random angular coordinates
		FUNCTION RND	Generation of quasi-random number
	SUBROUTINE EXPRO		Prediction of surface emission for external source of radiation
		FUNCTION BlackBodyFunction	Calculation of the Planck function for given parameters ω and T
	SUBROUTINE EMIT		Prediction of random direction of flight for each photon
		SUBROUTINE FI	Prediction of random angular coordinates
		FUNCTION RND	Generation of quasi-random number
	SUBROUTINE GEOMETRY		Calculation of coordinates of collisions of photon beam with surfaces of elementary calculation volumes
	SUBROUTINE RECYL		Registration of random events on cylindrical surface of calculation domain
	SUBROUTINE REGH		Registration of random events on plane surfaces of calculation domain
	SUBROUTINE SCAT		Simulation of photon scattering
		SUBROUTINE FI	Prediction of random angular coordinates
		FUNCTION RND	Generation of quasi-random number
	SUBROUTINE BIR		Interpretation of results of Monte-Carlo simulation

SUBROUTINE PROBT_Hybrid

Functional arrangement

SUBROUTINE PROBT_Hybrid			Monte-Carlo simulation with taking into account of rotational line structure (JLBL=2,3)
	SUBROUTINE MEAN		Averaging of temperatures (gas and solid/liquid phases) and optical properties inside elementary calculation zones (volumes)
		FUNCTION SUMAM	Integration of any function
	SUBROUTINE EXPELL		Prediction of volume emission of each elementary calculation volume
		FUNCTION BlackBodyFunction	Calculation of the Planck function for given parameters ω and T
	SUBROUTINE INCOOR		Prediction of initial spatial coordinate for each photon
		SUBROUTINE FI	Prediction of random angular coordinates
		FUNCTION RND	Generation of quasi-random number
	SUBROUTINE EXPRO		Prediction of surface emission for external source of radiation
		FUNCTION BlackBodyFunction	Calculation of the Planck function for given parameters ω and T
	SUBROUTINE EMIT		Prediction of random direction of flight for each photon
		SUBROUTINE FI	Prediction of random angular coordinates
		FUNCTION RND	Generation of quasi-random number
	SUBROUTINE BEAM_PARAMETERS		Calculation of temperature and optical properties in each point of photon beam
	SUBROUTINE RANDOM_FREE_PATH		Prediction of equivalent widths and averaged optical depths for photon beam. The random model of molecular lines is used here.
	SUBROUTINE RECYL		Registration of random events on cylindrical surface of calculation domain
	SUBROUTINE REGH		Registration of random events on plane surfaces of calculation domain
	SUBROUTINE SCAT		Simulation of photon scattering
		SUBROUTINE FI	Prediction of random angular coordinates
		SUBROUTINE RND	Generation of quasi-random number
	SUBROUTINE BIR		Interpretation of results of Monte-Carlo simulation